



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:37 PM UTC

PDB ID : 1XD4 / pdb_00001xd4
Title : Crystal structure of the DH-PH-cat module of Son of Sevenless (SOS)
Authors : Sondermann, H.; Soisson, S.M.; Boykevich, S.; Yang, S.S.; Bar-Sagi, D.; Kuriyan, J.
Deposited on : 2004-09-03
Resolution : 3.64 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

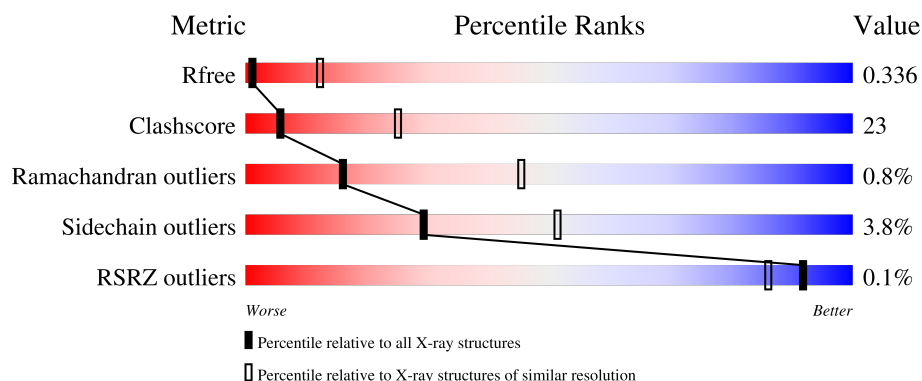
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.64 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1132 (3.76-3.52)
Clashscore	190562	1014 (3.74-3.54)
Ramachandran outliers	187476	1123 (3.76-3.52)
Sidechain outliers	187428	1121 (3.76-3.52)
RSRZ outliers	180081	1130 (3.76-3.52)

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

Mol	Chain	Length	Quality of chain
1	A	852	 64% 30% . .
1	B	852	 64% 30% . .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13542 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	824	Total	C	N	O	S	0	0	0
			6771	4323	1159	1258	31			
1	B	824	Total	C	N	O	S	0	0	0
			6771	4323	1159	1258	31			



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.47Å 127.36Å 279.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	11.99 – 3.64 11.99 – 3.64	Depositor EDS
% Data completeness (in resolution range)	92.0 (11.99-3.64) 89.1 (11.99-3.64)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 3.66Å)	Xtriage
Refinement program	CNS 1.1, REFMAC	Depositor
R, R_{free}	0.307 , 0.371 0.287 , 0.336	Depositor DCC
R_{free} test set	2033 reflections (6.90%)	wwPDB-VP
Wilson B-factor (Å ²)	131.1	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 111.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13542	wwPDB-VP
Average B, all atoms (Å ²)	154.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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	0.56	2/6918 (0.0%)	1.02	32/9334 (0.3%)
1	B	0.55	0/6918	1.04	41/9334 (0.4%)
All	All	0.56	2/13836 (0.0%)	1.03	73/18668 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	975	GLN	N-CA	5.38	1.52	1.46
1	A	974	TYR	CA-C	5.21	1.59	1.52

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	945	PRO	CA-N-CD	-16.63	88.72	112.00
1	A	580	PRO	CA-N-CD	-16.38	89.06	112.00
1	A	928	PRO	CA-N-CD	-14.69	91.44	112.00
1	B	972	GLN	OE1-CD-NE2	-10.46	112.14	122.60
1	B	977	GLN	OE1-CD-NE2	-10.27	112.33	122.60
1	A	977	GLN	OE1-CD-NE2	-10.11	112.49	122.60
1	B	426	GLN	OE1-CD-NE2	-10.00	112.60	122.60
1	A	972	GLN	OE1-CD-NE2	-9.89	112.71	122.60
1	B	375	GLN	OE1-CD-NE2	-9.85	112.75	122.60
1	B	314	GLN	OE1-CD-NE2	-9.82	112.78	122.60
1	A	500	GLN	OE1-CD-NE2	-9.81	112.79	122.60
1	B	755	GLN	OE1-CD-NE2	-9.79	112.81	122.60
1	B	566	GLN	OE1-CD-NE2	-9.78	112.82	122.60
1	A	973	GLN	OE1-CD-NE2	-9.77	112.83	122.60
1	A	975	GLN	OE1-CD-NE2	-9.77	112.83	122.60
1	A	545	GLN	OE1-CD-NE2	-9.76	112.84	122.60
1	B	975	GLN	OE1-CD-NE2	-9.74	112.86	122.60
1	A	426	GLN	OE1-CD-NE2	-9.68	112.92	122.60
1	A	570	PRO	CA-N-CD	-9.42	98.81	112.00
1	B	199	GLN	OE1-CD-NE2	-9.25	113.35	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	973	GLN	OE1-CD-NE2	-9.13	113.47	122.60
1	B	544	LEU	N-CA-C	-7.88	101.79	113.61
1	B	977	GLN	CG-CD-NE2	7.25	127.28	116.40
1	A	975	GLN	CG-CD-NE2	7.20	127.19	116.40
1	B	547	ARG	N-CA-C	-7.13	103.51	111.28
1	B	972	GLN	CG-CD-NE2	6.93	126.80	116.40
1	A	551	GLU	N-CA-C	-6.87	103.79	111.28
1	A	975	GLN	N-CA-C	6.83	118.80	111.36
1	A	545	GLN	CG-CD-NE2	6.83	126.64	116.40
1	A	973	GLN	CG-CD-NE2	6.78	126.57	116.40
1	A	977	GLN	CG-CD-NE2	6.68	126.42	116.40
1	B	314	GLN	CG-CD-NE2	6.67	126.41	116.40
1	B	755	GLN	CG-CD-NE2	6.67	126.40	116.40
1	B	1044	ASN	CA-C-N	6.66	128.17	119.84
1	B	1044	ASN	C-N-CA	6.66	128.17	119.84
1	B	375	GLN	CG-CD-NE2	6.65	126.38	116.40
1	B	566	GLN	CG-CD-NE2	6.64	126.37	116.40
1	A	500	GLN	CG-CD-NE2	6.64	126.36	116.40
1	B	973	GLN	CG-CD-NE2	6.60	126.30	116.40
1	A	972	GLN	CG-CD-NE2	6.55	126.23	116.40
1	A	631	TYR	N-CA-C	6.54	119.23	111.71
1	B	426	GLN	CG-CD-NE2	6.53	126.19	116.40
1	A	426	GLN	CG-CD-NE2	6.49	126.13	116.40
1	B	975	GLN	CG-CD-NE2	6.47	126.11	116.40
1	A	1044	ASN	CA-C-N	6.46	127.91	119.84
1	A	1044	ASN	C-N-CA	6.46	127.91	119.84
1	B	631	TYR	N-CA-C	6.46	119.14	111.71
1	B	520	ASP	CA-CB-CG	-6.19	106.41	112.60
1	B	461	ILE	N-CA-C	6.17	117.00	108.12
1	A	461	ILE	N-CA-C	6.05	116.83	108.12
1	A	394	SER	N-CA-C	5.99	118.29	111.11
1	B	559	LEU	N-CA-C	-5.95	106.11	113.19
1	B	394	SER	N-CA-C	5.95	118.25	111.11
1	B	199	GLN	CG-CD-NE2	5.86	125.19	116.40
1	B	873	GLU	N-CA-C	-5.80	104.55	111.69
1	A	682	ILE	N-CA-C	5.76	115.95	110.42
1	B	682	ILE	N-CA-C	5.75	115.94	110.42
1	B	617	MET	N-CA-C	5.67	118.31	111.40
1	A	617	MET	N-CA-C	5.65	118.29	111.40
1	A	1044	ASN	N-CA-C	5.56	119.33	108.21
1	B	1044	ASN	N-CA-C	5.52	119.24	108.21
1	A	225	VAL	N-CA-C	5.38	116.45	111.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	225	VAL	N-CA-C	5.38	116.45	111.45
1	A	307	PHE	N-CA-C	5.33	117.53	111.02
1	B	562	GLU	N-CA-C	-5.32	106.97	112.93
1	B	307	PHE	N-CA-C	5.29	117.48	111.02
1	A	223	ILE	N-CA-C	5.19	115.41	110.53
1	B	223	ILE	N-CA-C	5.18	115.40	110.53
1	B	467	LEU	N-CA-C	5.14	117.55	108.75
1	B	214	GLN	N-CA-C	-5.07	105.67	111.14
1	A	632	ARG	N-CA-C	5.04	118.53	112.38
1	B	632	ARG	N-CA-C	5.01	118.49	112.38
1	A	978	PRO	N-CA-C	5.00	119.16	111.21

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6771	0	6768	313	1
1	B	6771	0	6768	326	1
All	All	13542	0	13536	630	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (630) 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:626:THR:HG21	1:A:962:ARG:CD	1.57	1.35
1:B:584:GLU:CA	1:B:953:LYS:HG3	1.63	1.27
1:B:584:GLU:CB	1:B:953:LYS:HE3	1.68	1.24
1:A:587:ILE:HD13	1:A:603:ALA:CB	1.69	1.22
1:B:584:GLU:HA	1:B:953:LYS:CG	1.73	1.18
1:B:584:GLU:HB2	1:B:953:LYS:CE	1.74	1.15
1:A:587:ILE:CD1	1:A:603:ALA:HB3	1.77	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:ALA:HB2	1:A:948:LEU:HD12	1.26	1.12
1:B:584:GLU:HA	1:B:953:LYS:HG3	1.13	1.11
1:B:901:LEU:HG	1:B:905:HIS:CE1	1.86	1.10
1:A:626:THR:CG2	1:A:962:ARG:HD2	1.80	1.09
1:B:584:GLU:HB2	1:B:953:LYS:HE3	1.20	1.09
1:B:602:LYS:HE2	1:B:948:LEU:HD13	1.26	1.07
1:B:500:GLN:OE1	1:B:541:LEU:HB3	1.56	1.05
1:A:875:VAL:HG13	1:A:905:HIS:CD2	1.92	1.04
1:B:584:GLU:CB	1:B:953:LYS:HG3	1.89	1.01
1:A:496:MET:O	1:A:497:ARG:HG3	1.60	1.01
1:A:879:ASN:HD21	1:A:905:HIS:CD2	1.80	1.00
1:B:584:GLU:HB2	1:B:953:LYS:CD	1.91	0.99
1:B:341:ARG:NH2	1:B:536:ASN:HA	1.77	0.98
1:A:879:ASN:HD21	1:A:905:HIS:HD2	1.07	0.95
1:A:583:GLU:HB3	1:A:950:ARG:HD2	1.46	0.95
1:A:398:ARG:O	1:A:402:GLU:HG2	1.66	0.94
1:B:422:MET:HE3	1:B:437:ILE:HG22	1.50	0.94
1:A:317:LYS:HG2	1:A:318:PRO:HD2	1.48	0.93
1:A:422:MET:HE3	1:A:437:ILE:HG22	1.51	0.93
1:A:626:THR:CG2	1:A:962:ARG:HG2	1.99	0.93
1:B:875:VAL:HG13	1:B:905:HIS:CD2	2.04	0.93
1:A:587:ILE:HD11	1:A:955:LEU:HD12	1.48	0.92
1:B:630:THR:HG22	1:B:805:VAL:HG21	1.49	0.92
1:B:604:GLY:HA2	1:B:955:LEU:HD12	1.51	0.92
1:A:603:ALA:CB	1:A:948:LEU:HD12	2.00	0.92
1:B:796:TYR:OH	1:B:971:ILE:HG23	1.70	0.91
1:A:428:ASN:HD21	1:A:487:GLU:H	1.16	0.91
1:A:317:LYS:CG	1:A:318:PRO:HD2	2.01	0.91
1:B:796:TYR:CE2	1:B:975:GLN:HG2	2.05	0.91
1:A:330:GLY:HA3	1:A:546:TYR:CE2	2.07	0.90
1:B:628:LEU:HD12	1:B:695:HIS:HD2	1.37	0.88
1:B:716:GLU:O	1:B:720:THR:HG23	1.72	0.88
1:B:796:TYR:CE2	1:B:975:GLN:CG	2.57	0.88
1:A:716:GLU:O	1:A:720:THR:HG23	1.72	0.88
1:B:875:VAL:HG13	1:B:905:HIS:HD2	1.38	0.88
1:B:602:LYS:HE2	1:B:948:LEU:CD1	2.04	0.87
1:A:341:ARG:NH2	1:A:536:ASN:HA	1.89	0.87
1:A:628:LEU:HD12	1:A:695:HIS:HD2	1.37	0.87
1:A:919:LEU:HD11	1:A:928:PRO:HG3	1.56	0.87
1:A:919:LEU:CD1	1:A:928:PRO:HG3	2.05	0.87
1:B:269:MET:SD	1:B:729:TRP:CD1	2.68	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:584:GLU:HA	1:B:953:LYS:CB	2.04	0.86
1:A:428:ASN:ND2	1:A:487:GLU:H	1.72	0.86
1:B:630:THR:HG22	1:B:805:VAL:CG2	2.05	0.86
1:A:626:THR:HG22	1:A:958:PHE:CE2	2.10	0.86
1:B:915:TYR:CZ	1:B:929:PHE:HB3	2.10	0.86
1:A:499:VAL:HG12	1:A:501:ILE:CD1	2.06	0.85
1:B:428:ASN:ND2	1:B:487:GLU:H	1.73	0.85
1:B:398:ARG:O	1:B:402:GLU:HG3	1.75	0.85
1:A:626:THR:HG21	1:A:962:ARG:CG	2.07	0.85
1:B:499:VAL:HG12	1:B:501:ILE:CD1	2.06	0.85
1:A:626:THR:HG21	1:A:962:ARG:HD2	0.86	0.85
1:B:330:GLY:HA3	1:B:546:TYR:CE2	2.11	0.84
1:A:946:GLU:HG3	1:A:947:VAL:HG13	1.57	0.84
1:B:428:ASN:HD21	1:B:487:GLU:H	1.24	0.84
1:A:576:ARG:HD3	1:A:646:GLU:OE2	1.78	0.83
1:B:304:ARG:HD3	1:B:310:ARG:HH12	1.42	0.83
1:B:584:GLU:HB3	1:B:953:LYS:HE3	1.57	0.83
1:A:926:CYS:HA	1:A:979:TYR:OH	1.77	0.83
1:B:576:ARG:HD3	1:B:646:GLU:OE2	1.78	0.83
1:A:901:LEU:CD1	1:A:905:HIS:CE1	2.61	0.82
1:A:626:THR:CG2	1:A:962:ARG:CG	2.56	0.82
1:A:626:THR:HG22	1:A:958:PHE:HE2	1.41	0.82
1:A:810:THR:HA	1:B:1001:MET:HE3	1.61	0.82
1:B:629:THR:HG23	1:B:801:PRO:HB2	1.62	0.81
1:B:824:MET:HE1	1:B:930:PHE:CE2	2.15	0.81
1:B:341:ARG:NH2	1:B:536:ASN:CA	2.43	0.81
1:B:629:THR:HG23	1:B:801:PRO:CB	2.11	0.81
1:A:446:MET:HE2	1:A:540:ALA:HB3	1.63	0.81
1:A:828:THR:HG23	1:A:873:GLU:HG2	1.61	0.80
1:B:828:THR:HG23	1:B:873:GLU:HG2	1.64	0.80
1:B:584:GLU:CB	1:B:953:LYS:CG	2.59	0.80
1:B:901:LEU:CG	1:B:905:HIS:CE1	2.63	0.80
1:A:901:LEU:HD11	1:A:905:HIS:CE1	2.16	0.80
1:B:225:VAL:HG21	1:B:554:LEU:HB2	1.61	0.80
1:B:584:GLU:CB	1:B:953:LYS:CE	2.44	0.80
1:A:901:LEU:CD1	1:A:905:HIS:HE1	1.95	0.80
1:A:587:ILE:O	1:A:602:LYS:HB3	1.82	0.80
1:A:317:LYS:CG	1:A:318:PRO:CD	2.61	0.79
1:A:587:ILE:N	1:A:587:ILE:HD12	1.98	0.79
1:B:337:TYR:OH	1:B:502:ASN:ND2	2.15	0.79
1:A:583:GLU:O	1:A:950:ARG:HB3	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:MET:O	1:A:497:ARG:CG	2.31	0.78
1:B:330:GLY:CA	1:B:546:TYR:CE2	2.67	0.77
1:A:901:LEU:HG	1:A:905:HIS:CE1	2.20	0.77
1:A:499:VAL:CG1	1:A:501:ILE:CD1	2.63	0.77
1:A:500:GLN:NE2	1:A:538:MET:SD	2.58	0.76
1:B:584:GLU:CB	1:B:953:LYS:CD	2.62	0.76
1:B:628:LEU:HD12	1:B:695:HIS:CD2	2.20	0.76
1:A:500:GLN:HE22	1:A:538:MET:CE	1.98	0.76
1:A:626:THR:CG2	1:A:962:ARG:CD	2.49	0.76
1:A:628:LEU:HD12	1:A:695:HIS:CD2	2.20	0.76
1:B:499:VAL:CG1	1:B:501:ILE:CD1	2.63	0.76
1:B:446:MET:HE1	1:B:537:TRP:HA	1.68	0.76
1:A:634:PHE:CE2	1:A:958:PHE:HD1	2.05	0.75
1:B:271:ASP:OD2	1:B:695:HIS:HB2	1.86	0.75
1:A:634:PHE:CE2	1:A:958:PHE:CD1	2.74	0.75
1:A:317:LYS:HG2	1:A:318:PRO:CD	2.16	0.75
1:A:446:MET:HE1	1:A:537:TRP:HA	1.68	0.75
1:B:804:LEU:HD23	1:B:968:THR:HG22	1.68	0.75
1:B:582:SER:OG	1:B:584:GLU:HG2	1.86	0.75
1:A:520:ASP:OD1	1:A:520:ASP:O	2.05	0.75
1:A:587:ILE:HD11	1:A:955:LEU:CD1	2.16	0.75
1:A:502:ASN:HD21	1:A:534:LYS:NZ	1.85	0.74
1:B:202:TYR:CE2	1:B:206:LYS:HD3	2.22	0.74
1:B:831:LEU:HD23	1:B:873:GLU:OE1	1.87	0.74
1:B:604:GLY:N	1:B:955:LEU:HB3	2.02	0.74
1:A:926:CYS:SG	1:A:928:PRO:HD2	2.28	0.74
1:B:584:GLU:CA	1:B:953:LYS:CG	2.44	0.74
1:A:831:LEU:HD23	1:A:873:GLU:OE1	1.87	0.74
1:A:202:TYR:CE2	1:A:206:LYS:HD3	2.22	0.74
1:A:500:GLN:NE2	1:A:538:MET:CE	2.50	0.74
1:B:547:ARG:O	1:B:551:GLU:HG2	1.88	0.74
1:B:1018:PRO:HB3	1:B:1022:LYS:HD3	1.69	0.73
1:B:603:ALA:HA	1:B:956:ILE:O	1.88	0.73
1:B:449:THR:HG21	1:B:458:GLU:OE1	1.89	0.73
1:A:925:PRO:HG2	1:A:978:PRO:O	1.89	0.73
1:A:449:THR:HG21	1:A:458:GLU:OE1	1.89	0.73
1:A:1018:PRO:HB3	1:A:1022:LYS:HD3	1.69	0.72
1:A:422:MET:CE	1:A:437:ILE:HG22	2.20	0.72
1:A:500:GLN:NE2	1:A:538:MET:HE1	2.03	0.72
1:B:221:LEU:HA	1:B:554:LEU:HD22	1.71	0.72
1:A:626:THR:CG2	1:A:958:PHE:HE2	2.03	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:LEU:HD11	1:A:905:HIS:HE1	1.51	0.71
1:A:207:ALA:O	1:A:211:GLU:HG3	1.91	0.71
1:B:901:LEU:HD11	1:B:905:HIS:NE2	2.06	0.71
1:B:207:ALA:O	1:B:211:GLU:HG3	1.91	0.71
1:B:626:THR:HG21	1:B:958:PHE:CZ	2.25	0.71
1:B:796:TYR:HE2	1:B:975:GLN:CG	2.03	0.71
1:B:614:THR:OG1	1:B:647:ARG:HD3	1.90	0.71
1:A:614:THR:OG1	1:A:647:ARG:HD3	1.90	0.70
1:A:901:LEU:CG	1:A:905:HIS:HE1	2.03	0.70
1:A:507:THR:C	1:A:509:GLU:H	1.99	0.70
1:B:199:GLN:HB3	1:B:203:ASP:HB2	1.72	0.70
1:B:341:ARG:HH22	1:B:536:ASN:N	1.88	0.70
1:B:912:TYR:HB2	1:B:932:ILE:HD11	1.72	0.70
1:B:916:LEU:HD21	1:B:932:ILE:HG21	1.73	0.70
1:B:507:THR:C	1:B:509:GLU:H	1.99	0.70
1:B:422:MET:CE	1:B:437:ILE:HG22	2.20	0.70
1:A:480:LEU:HD12	1:A:481:PRO:HD2	1.71	0.70
1:A:859:LEU:HD11	1:A:871:VAL:HG13	1.74	0.70
1:B:809:TRP:HH2	1:B:937:ILE:HG22	1.55	0.70
1:B:947:VAL:HG21	1:B:954:GLU:HG3	1.74	0.70
1:B:419:ILE:HG22	1:B:419:ILE:O	1.91	0.69
1:A:419:ILE:HG22	1:A:419:ILE:O	1.91	0.69
1:A:912:TYR:CD2	1:A:932:ILE:HD11	2.27	0.69
1:A:585:ASN:HA	1:A:955:LEU:HD22	1.75	0.69
1:B:268:GLU:OE1	1:B:688:ARG:NH2	2.25	0.69
1:A:330:GLY:CA	1:A:546:TYR:CE2	2.75	0.69
1:A:958:PHE:CE2	1:A:962:ARG:HG2	2.28	0.69
1:B:796:TYR:HE2	1:B:975:GLN:HG2	1.58	0.68
1:A:355:GLU:HG3	1:A:359:GLN:HE21	1.58	0.68
1:A:496:MET:C	1:A:497:ARG:HG3	2.17	0.68
1:B:225:VAL:CG2	1:B:554:LEU:HB2	2.22	0.68
1:A:500:GLN:OE1	1:A:541:LEU:HB2	1.94	0.68
1:B:341:ARG:HH21	1:B:536:ASN:HA	1.58	0.68
1:A:879:ASN:ND2	1:A:905:HIS:CD2	2.60	0.68
1:A:539:ALA:O	1:A:543:SER:HB2	1.94	0.68
1:A:587:ILE:HD13	1:A:603:ALA:HB3	0.81	0.68
1:A:276:HIS:HE1	1:A:365:GLU:H	1.42	0.68
1:A:881:SER:OG	1:B:881:SER:N	2.27	0.67
1:B:355:GLU:HG3	1:B:359:GLN:HE21	1.58	0.67
1:A:502:ASN:HD21	1:A:534:LYS:HZ3	1.43	0.67
1:B:446:MET:HE2	1:B:540:ALA:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ARG:HG3	1:A:403:SER:OG	1.95	0.67
1:B:276:HIS:HE1	1:B:365:GLU:H	1.42	0.67
1:A:881:SER:N	1:B:881:SER:OG	2.28	0.67
1:B:498:LYS:HD2	1:B:517:ILE:O	1.95	0.67
1:B:341:ARG:HG3	1:B:403:SER:OG	1.95	0.66
1:B:954:GLU:C	1:B:955:LEU:HD22	2.20	0.66
1:A:226:PHE:HZ	1:A:550:LEU:HD13	1.61	0.66
1:B:947:VAL:HB	1:B:955:LEU:O	1.94	0.66
1:B:999:ASN:C	1:B:999:ASN:HD22	2.02	0.66
1:B:445:ILE:HD13	1:B:544:LEU:HD23	1.78	0.66
1:A:999:ASN:C	1:A:999:ASN:HD22	2.02	0.66
1:B:341:ARG:NH2	1:B:536:ASN:OD1	2.28	0.66
1:A:499:VAL:HG12	1:A:501:ILE:HD12	1.78	0.66
1:A:498:LYS:HD2	1:A:517:ILE:O	1.95	0.66
1:A:901:LEU:CG	1:A:905:HIS:CE1	2.78	0.66
1:B:585:ASN:C	1:B:955:LEU:HD11	2.21	0.66
1:B:630:THR:CA	1:B:805:VAL:HG11	2.26	0.65
1:B:237:PHE:HD1	1:B:314:GLN:OE1	1.78	0.65
1:A:269:MET:SD	1:A:729:TRP:CD1	2.89	0.65
1:B:872:LEU:N	1:B:872:LEU:CD2	2.60	0.65
1:A:1044:ASN:N	1:A:1045:PRO:HD3	2.12	0.65
1:B:926:CYS:O	1:B:928:PRO:HD3	1.96	0.65
1:A:444:PHE:HZ	1:A:447:GLU:HB2	1.62	0.65
1:B:901:LEU:CD1	1:B:905:HIS:NE2	2.60	0.65
1:B:872:LEU:N	1:B:872:LEU:HD23	2.12	0.64
1:A:926:CYS:SG	1:A:928:PRO:CD	2.85	0.64
1:B:444:PHE:HZ	1:B:447:GLU:HB2	1.62	0.64
1:B:1044:ASN:N	1:B:1045:PRO:HD3	2.12	0.64
1:A:446:MET:HE2	1:A:540:ALA:CB	2.27	0.64
1:B:796:TYR:CE2	1:B:975:GLN:HG3	2.31	0.64
1:A:226:PHE:CZ	1:A:550:LEU:HD13	2.33	0.64
1:B:584:GLU:HA	1:B:953:LYS:HB3	1.80	0.64
1:A:586:ILE:HD11	1:A:601:ILE:HG13	1.78	0.64
1:B:445:ILE:CD1	1:B:544:LEU:HD23	2.27	0.64
1:A:796:TYR:CD1	1:A:930:PHE:HD2	2.16	0.64
1:B:459:ARG:HH11	1:B:459:ARG:HG2	1.63	0.64
1:B:330:GLY:HA3	1:B:546:TYR:CD2	2.34	0.63
1:B:584:GLU:HB2	1:B:953:LYS:HD2	1.77	0.63
1:A:480:LEU:CD1	1:A:481:PRO:HD2	2.27	0.63
1:A:499:VAL:CG1	1:A:501:ILE:HD11	2.28	0.63
1:B:901:LEU:HG	1:B:905:HIS:HE1	1.53	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ARG:HG2	1:A:459:ARG:HH11	1.63	0.63
1:A:919:LEU:HD13	1:A:928:PRO:HG3	1.81	0.63
1:B:341:ARG:HH12	1:B:535:ASN:HB3	1.63	0.63
1:A:499:VAL:HG11	1:A:501:ILE:HD11	1.80	0.63
1:A:585:ASN:ND2	1:A:586:ILE:HG22	2.14	0.63
1:A:797:ARG:NH1	1:A:975:GLN:O	2.31	0.63
1:B:869:ASN:O	1:B:873:GLU:HG3	1.99	0.63
1:A:788:LEU:HD13	1:A:831:LEU:HD21	1.81	0.62
1:B:499:VAL:CG1	1:B:501:ILE:HD11	2.28	0.62
1:B:584:GLU:HB3	1:B:953:LYS:HG3	1.79	0.62
1:B:957:ASN:OD1	1:B:960:LYS:HB2	1.97	0.62
1:B:499:VAL:HG11	1:B:501:ILE:HD11	1.80	0.62
1:B:809:TRP:HH2	1:B:937:ILE:CG2	2.11	0.62
1:B:859:LEU:HD11	1:B:871:VAL:HG13	1.82	0.62
1:B:237:PHE:CD1	1:B:314:GLN:OE1	2.53	0.62
1:B:499:VAL:HG12	1:B:501:ILE:HD12	1.78	0.62
1:A:869:ASN:O	1:A:873:GLU:HG3	1.99	0.62
1:B:224:LYS:HB3	1:B:557:THR:HG21	1.82	0.62
1:B:269:MET:SD	1:B:729:TRP:NE1	2.72	0.62
1:A:317:LYS:HG3	1:A:318:PRO:HD2	1.79	0.62
1:B:445:ILE:HD11	1:B:544:LEU:CD2	2.30	0.62
1:B:1003:LYS:HE3	1:B:1003:LYS:HA	1.82	0.62
1:B:630:THR:CB	1:B:805:VAL:HG11	2.29	0.62
1:A:317:LYS:HG3	1:A:318:PRO:CD	2.29	0.61
1:B:496:MET:O	1:B:497:ARG:CG	2.48	0.61
1:B:672:ALA:O	1:B:676:ARG:HG3	2.00	0.61
1:A:630:THR:HG22	1:A:965:ALA:HB2	1.82	0.61
1:A:364:SER:HB3	1:A:370:LYS:HG2	1.83	0.61
1:A:450:LEU:HD12	1:A:461:ILE:HD12	1.83	0.61
1:A:672:ALA:O	1:A:676:ARG:HG3	2.00	0.61
1:B:450:LEU:HD12	1:B:461:ILE:HD12	1.83	0.61
1:A:586:ILE:HA	1:A:603:ALA:O	2.01	0.61
1:A:866:ASN:HB3	1:A:926:CYS:HB2	1.83	0.61
1:B:367:GLN:O	1:B:371:GLU:HG2	2.01	0.61
1:A:202:TYR:O	1:A:206:LYS:HG3	2.00	0.61
1:A:540:ALA:O	1:A:544:LEU:HB2	2.01	0.61
1:B:788:LEU:HD13	1:B:831:LEU:HD21	1.81	0.61
1:A:367:GLN:O	1:A:371:GLU:HG2	2.01	0.61
1:B:364:SER:HB3	1:B:370:LYS:HG2	1.83	0.61
1:B:540:ALA:O	1:B:544:LEU:HB2	2.01	0.60
1:A:1003:LYS:HE3	1:A:1003:LYS:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:645:ILE:O	1:B:649:GLU:HG2	2.01	0.60
1:A:260:LEU:HD22	1:A:264:GLU:HG3	1.83	0.60
1:A:269:MET:CE	1:A:729:TRP:CD1	2.84	0.60
1:A:645:ILE:O	1:A:649:GLU:HG2	2.01	0.60
1:B:260:LEU:HD22	1:B:264:GLU:HG3	1.83	0.60
1:B:446:MET:HE3	1:B:463:LEU:HD12	1.83	0.60
1:A:337:TYR:CD2	1:A:538:MET:CB	2.84	0.60
1:A:587:ILE:O	1:A:602:LYS:N	2.33	0.60
1:A:796:TYR:HD1	1:A:930:PHE:HD2	1.49	0.60
1:B:202:TYR:O	1:B:206:LYS:HG3	2.01	0.60
1:B:539:ALA:O	1:B:543:SER:HB3	2.01	0.60
1:B:364:SER:HB3	1:B:370:LYS:CG	2.31	0.60
1:B:584:GLU:OE1	1:B:953:LYS:HE3	2.02	0.60
1:A:364:SER:HB3	1:A:370:LYS:CG	2.32	0.60
1:B:564:GLU:HB2	1:B:676:ARG:NH1	2.16	0.60
1:B:496:MET:O	1:B:497:ARG:HG3	2.01	0.60
1:B:630:THR:HB	1:B:805:VAL:HG11	1.83	0.59
1:A:539:ALA:O	1:A:543:SER:CB	2.50	0.59
1:B:330:GLY:HA2	1:B:546:TYR:CE2	2.37	0.59
1:B:445:ILE:HD11	1:B:544:LEU:HD21	1.83	0.59
1:B:807:SER:OG	1:B:941:GLU:CG	2.51	0.59
1:B:807:SER:OG	1:B:941:GLU:HG3	2.02	0.59
1:B:824:MET:HE1	1:B:930:PHE:CD2	2.37	0.59
1:A:925:PRO:CG	1:A:978:PRO:O	2.50	0.59
1:B:260:LEU:O	1:B:264:GLU:HG3	2.03	0.59
1:B:603:ALA:HB1	1:B:955:LEU:CB	2.33	0.59
1:A:796:TYR:CD1	1:A:930:PHE:CD2	2.90	0.59
1:A:446:MET:HE3	1:A:463:LEU:HD12	1.83	0.58
1:A:500:GLN:OE1	1:A:541:LEU:CB	2.50	0.58
1:B:946:GLU:HG3	1:B:947:VAL:HG13	1.83	0.58
1:A:260:LEU:O	1:A:264:GLU:HG3	2.03	0.58
1:A:958:PHE:CE2	1:A:962:ARG:CG	2.86	0.58
1:B:221:LEU:CA	1:B:554:LEU:HD22	2.32	0.58
1:B:245:ILE:HD11	1:B:314:GLN:HG2	1.85	0.58
1:A:587:ILE:HD12	1:A:587:ILE:H	1.67	0.58
1:A:269:MET:HE1	1:A:729:TRP:CD1	2.38	0.58
1:B:560:GLN:C	1:B:562:GLU:H	2.10	0.58
1:B:926:CYS:HA	1:B:979:TYR:OH	2.03	0.58
1:B:445:ILE:CD1	1:B:544:LEU:CD2	2.81	0.58
1:B:498:LYS:HB3	1:B:517:ILE:O	2.04	0.58
1:A:337:TYR:CD2	1:A:538:MET:HB3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:630:THR:HA	1:B:805:VAL:HG11	1.86	0.58
1:B:901:LEU:CD1	1:B:905:HIS:CE1	2.86	0.58
1:A:276:HIS:CE1	1:A:365:GLU:H	2.22	0.58
1:B:890:PHE:O	1:B:898:LYS:HE2	2.04	0.58
1:A:824:MET:HE1	1:A:930:PHE:CG	2.39	0.57
1:A:890:PHE:O	1:A:898:LYS:HE2	2.04	0.57
1:A:498:LYS:HB3	1:A:517:ILE:O	2.04	0.57
1:A:950:ARG:HB2	1:A:955:LEU:HD11	1.87	0.57
1:A:537:TRP:O	1:A:541:LEU:HG	2.03	0.57
1:A:796:TYR:CE1	1:A:930:PHE:CD2	2.92	0.57
1:B:341:ARG:NH2	1:B:536:ASN:N	2.51	0.57
1:B:875:VAL:CG1	1:B:905:HIS:HD2	2.12	0.57
1:B:958:PHE:C	1:B:960:LYS:H	2.12	0.57
1:A:549:THR:O	1:A:552:ARG:HB3	2.05	0.56
1:A:634:PHE:CZ	1:A:958:PHE:CD1	2.92	0.56
1:B:809:TRP:CH2	1:B:937:ILE:CG2	2.88	0.56
1:B:498:LYS:HD3	1:B:499:VAL:H	1.71	0.56
1:B:583:GLU:OE2	1:B:950:ARG:HB3	2.05	0.56
1:A:445:ILE:HD13	1:A:544:LEU:HD23	1.88	0.56
1:A:976:ASN:O	1:A:978:PRO:HD3	2.06	0.56
1:B:626:THR:CG2	1:B:958:PHE:CZ	2.89	0.55
1:B:629:THR:HG23	1:B:801:PRO:HB3	1.86	0.55
1:B:276:HIS:CE1	1:B:365:GLU:H	2.22	0.55
1:A:479:ARG:HG2	1:A:479:ARG:HH11	1.71	0.55
1:B:479:ARG:HG2	1:B:479:ARG:HH11	1.72	0.55
1:A:866:ASN:O	1:A:926:CYS:HB2	2.06	0.55
1:A:341:ARG:NH2	1:A:536:ASN:CA	2.66	0.55
1:A:498:LYS:HD3	1:A:499:VAL:H	1.71	0.55
1:B:915:TYR:OH	1:B:929:PHE:N	2.39	0.55
1:B:201:TYR:O	1:B:205:VAL:HG23	2.07	0.55
1:B:224:LYS:NZ	1:B:558:MET:HG2	2.22	0.55
1:A:694:ARG:O	1:A:698:GLU:HB2	2.07	0.54
1:B:582:SER:H	1:B:585:ASN:HD21	1.54	0.54
1:B:694:ARG:O	1:B:698:GLU:HB2	2.07	0.54
1:B:919:LEU:HD12	1:B:922:ILE:HD11	1.88	0.54
1:A:445:ILE:CD1	1:A:544:LEU:HD23	2.38	0.54
1:A:544:LEU:HD13	1:A:544:LEU:O	2.08	0.54
1:B:938:LEU:O	1:B:942:GLU:HG2	2.07	0.54
1:A:587:ILE:O	1:A:602:LYS:CB	2.54	0.54
1:B:330:GLY:CA	1:B:546:TYR:HE2	2.20	0.54
1:B:330:GLY:HA3	1:B:546:TYR:HE2	1.69	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:THR:O	1:B:509:GLU:N	2.40	0.54
1:A:585:ASN:OD1	1:A:608:LYS:HE3	2.08	0.54
1:B:604:GLY:O	1:B:956:ILE:HG12	2.08	0.54
1:A:507:THR:O	1:A:509:GLU:N	2.40	0.53
1:A:500:GLN:HE21	1:A:538:MET:HE1	1.73	0.53
1:B:727:LYS:O	1:B:731:GLU:HG2	2.09	0.53
1:B:809:TRP:CH2	1:B:937:ILE:HG22	2.41	0.53
1:A:587:ILE:N	1:A:603:ALA:O	2.34	0.53
1:B:507:THR:C	1:B:509:GLU:N	2.67	0.52
1:B:544:LEU:HD13	1:B:544:LEU:O	2.10	0.52
1:A:269:MET:HG3	1:A:691:ASN:OD1	2.10	0.52
1:B:912:TYR:CE1	1:B:929:PHE:CE2	2.98	0.52
1:B:915:TYR:OH	1:B:929:PHE:HB3	2.08	0.52
1:A:311:PHE:O	1:A:315:LEU:HD13	2.09	0.52
1:A:626:THR:HG23	1:A:962:ARG:HG2	1.89	0.52
1:A:872:LEU:HD12	1:A:929:PHE:CG	2.45	0.52
1:A:950:ARG:C	1:A:952:GLY:H	2.17	0.52
1:B:500:GLN:C	1:B:501:ILE:HD12	2.35	0.52
1:A:810:THR:HB	1:B:999:ASN:O	2.09	0.51
1:B:221:LEU:CD1	1:B:554:LEU:HD22	2.40	0.51
1:B:585:ASN:C	1:B:955:LEU:CD1	2.83	0.51
1:B:933:TYR:O	1:B:937:ILE:HG13	2.10	0.51
1:B:796:TYR:HE2	1:B:975:GLN:HG3	1.73	0.51
1:A:500:GLN:C	1:A:501:ILE:HD12	2.35	0.51
1:B:585:ASN:CA	1:B:955:LEU:HD11	2.40	0.51
1:A:543:SER:O	1:A:547:ARG:HB3	2.11	0.51
1:A:474:ASN:HB2	1:A:479:ARG:HH21	1.75	0.51
1:A:630:THR:CG2	1:A:965:ALA:HB2	2.40	0.51
1:B:603:ALA:C	1:B:955:LEU:HB3	2.35	0.51
1:A:506:ASP:C	1:A:508:ASN:N	2.68	0.51
1:B:311:PHE:O	1:B:315:LEU:HD13	2.10	0.51
1:B:610:ILE:HD12	1:B:643:LEU:HD13	1.93	0.51
1:A:553:MET:HA	1:A:553:MET:HE2	1.92	0.51
1:A:630:THR:OG1	1:A:958:PHE:CZ	2.64	0.51
1:A:899:LYS:O	1:A:903:GLU:HG2	2.11	0.51
1:B:899:LYS:O	1:B:903:GLU:HG2	2.11	0.51
1:B:552:ARG:O	1:B:556:VAL:HG23	2.11	0.51
1:A:499:VAL:HG12	1:A:500:GLN:N	2.26	0.50
1:B:585:ASN:C	1:B:585:ASN:HD22	2.19	0.50
1:A:912:TYR:CG	1:A:932:ILE:HD11	2.45	0.50
1:B:771:ILE:HG22	1:B:986:ASP:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:PHE:CE2	1:A:958:PHE:CE1	2.99	0.50
1:B:304:ARG:HD3	1:B:310:ARG:NH1	2.20	0.50
1:B:988:LYS:O	1:B:992:GLU:HG3	2.11	0.50
1:A:568:ARG:HH12	1:A:656:THR:HG22	1.77	0.50
1:B:446:MET:HE2	1:B:540:ALA:CB	2.41	0.50
1:B:499:VAL:HG12	1:B:500:GLN:N	2.26	0.50
1:B:866:ASN:HB3	1:B:926:CYS:HB2	1.93	0.50
1:A:468:MET:HE1	1:A:516:ILE:HD12	1.94	0.50
1:B:763:TRP:CE2	1:B:768:PRO:HG3	2.47	0.50
1:A:480:LEU:CG	1:A:481:PRO:HD2	2.41	0.50
1:A:584:GLU:O	1:A:955:LEU:HD21	2.11	0.50
1:A:628:LEU:CD1	1:A:695:HIS:HD2	2.15	0.50
1:A:912:TYR:CE2	1:A:932:ILE:HD11	2.47	0.50
1:A:988:LYS:O	1:A:992:GLU:HG3	2.11	0.50
1:B:474:ASN:HB2	1:B:479:ARG:HH21	1.75	0.50
1:B:628:LEU:CD1	1:B:695:HIS:HD2	2.15	0.50
1:B:955:LEU:HD22	1:B:955:LEU:N	2.27	0.50
1:A:445:ILE:HD11	1:A:544:LEU:CD2	2.42	0.49
1:A:507:THR:C	1:A:509:GLU:N	2.68	0.49
1:B:539:ALA:O	1:B:543:SER:CB	2.61	0.49
1:B:506:ASP:C	1:B:508:ASN:N	2.68	0.49
1:B:977:GLN:OE1	1:B:977:GLN:N	2.44	0.49
1:A:446:MET:CE	1:A:463:LEU:HD12	2.42	0.49
1:A:771:ILE:HG22	1:A:986:ASP:HB3	1.95	0.49
1:B:399:ARG:O	1:B:402:GLU:HB2	2.13	0.49
1:B:558:MET:C	1:B:560:GLN:H	2.21	0.49
1:B:306:GLY:O	1:B:310:ARG:HD2	2.13	0.49
1:B:468:MET:HE1	1:B:516:ILE:HD12	1.94	0.49
1:A:269:MET:CE	1:A:729:TRP:HD1	2.25	0.49
1:A:480:LEU:HG	1:A:481:PRO:HD2	1.95	0.49
1:A:610:ILE:HD12	1:A:643:LEU:HD13	1.93	0.49
1:A:763:TRP:CE2	1:A:768:PRO:HG3	2.47	0.49
1:A:445:ILE:HD11	1:A:544:LEU:HD21	1.94	0.48
1:A:824:MET:HE1	1:A:930:PHE:CD2	2.47	0.48
1:A:419:ILE:O	1:A:419:ILE:CG2	2.60	0.48
1:A:474:ASN:CB	1:A:479:ARG:HH21	2.26	0.48
1:B:1030:LYS:HD2	1:B:1031:TYR:CZ	2.48	0.48
1:A:796:TYR:CE1	1:A:930:PHE:CE2	3.01	0.48
1:A:866:ASN:HB3	1:A:926:CYS:CB	2.43	0.48
1:B:446:MET:CE	1:B:463:LEU:HD12	2.43	0.48
1:A:337:TYR:CD2	1:A:538:MET:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:ASN:ND2	1:A:534:LYS:NZ	2.59	0.48
1:B:603:ALA:CB	1:B:955:LEU:HB2	2.44	0.48
1:A:217:ARG:HH12	1:A:554:LEU:HD23	1.79	0.48
1:A:468:MET:HE1	1:A:516:ILE:CD1	2.44	0.48
1:A:578:ALA:O	1:A:579:GLU:C	2.54	0.48
1:A:587:ILE:HD12	1:A:603:ALA:O	2.14	0.48
1:A:1030:LYS:HD2	1:A:1031:TYR:CZ	2.48	0.48
1:B:630:THR:HG22	1:B:805:VAL:HG22	1.92	0.48
1:B:468:MET:HE1	1:B:516:ILE:CD1	2.44	0.48
1:B:474:ASN:CB	1:B:479:ARG:HH21	2.27	0.48
1:A:568:ARG:NH1	1:A:656:THR:HG22	2.29	0.48
1:B:875:VAL:HG22	1:B:905:HIS:CD2	2.49	0.48
1:A:449:THR:CG2	1:A:458:GLU:OE1	2.61	0.48
1:B:958:PHE:C	1:B:960:LYS:N	2.71	0.48
1:A:587:ILE:HG13	1:A:950:ARG:HG3	1.96	0.47
1:B:260:LEU:HD22	1:B:264:GLU:CG	2.44	0.47
1:A:399:ARG:O	1:A:402:GLU:HB2	2.14	0.47
1:A:634:PHE:CZ	1:A:958:PHE:HD1	2.31	0.47
1:A:562:GLU:HG2	1:A:562:GLU:O	2.15	0.47
1:A:926:CYS:SG	1:A:928:PRO:HD3	2.54	0.47
1:A:245:ILE:HD11	1:A:314:GLN:HG2	1.96	0.47
1:A:341:ARG:NH2	1:A:536:ASN:OD1	2.47	0.47
1:A:445:ILE:CD1	1:A:544:LEU:CD2	2.92	0.47
1:A:654:GLU:HG2	1:A:655:PRO:HD2	1.95	0.47
1:B:603:ALA:CB	1:B:955:LEU:CB	2.92	0.47
1:B:922:ILE:HD12	1:B:922:ILE:O	2.13	0.47
1:B:947:VAL:CB	1:B:955:LEU:O	2.60	0.47
1:A:528:ALA:HB1	1:A:533:GLU:HB3	1.97	0.47
1:A:567:MET:SD	1:A:567:MET:N	2.87	0.47
1:B:458:GLU:O	1:B:458:GLU:HG3	2.13	0.47
1:A:228:GLU:OE1	1:A:228:GLU:HA	2.15	0.47
1:A:634:PHE:HE2	1:A:958:PHE:CD1	2.26	0.47
1:B:585:ASN:HD22	1:B:586:ILE:N	2.13	0.47
1:A:668:GLN:HA	1:A:669:PRO:HD3	1.82	0.47
1:B:228:GLU:HA	1:B:228:GLU:OE1	2.15	0.47
1:B:560:GLN:C	1:B:562:GLU:N	2.74	0.46
1:A:421:LYS:O	1:A:425:ILE:HG13	2.15	0.46
1:A:217:ARG:HG3	1:A:217:ARG:HH11	1.80	0.46
1:A:770:HIS:HA	1:A:772:GLU:OE2	2.15	0.46
1:B:528:ALA:HB1	1:B:533:GLU:HB3	1.97	0.46
1:B:629:THR:CG2	1:B:801:PRO:HB3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:TYR:CD1	1:B:510:TYR:O	2.69	0.46
1:A:458:GLU:O	1:A:458:GLU:HG3	2.14	0.46
1:A:510:TYR:O	1:A:510:TYR:CD1	2.69	0.46
1:A:587:ILE:CD1	1:A:603:ALA:CB	2.61	0.46
1:A:949:LYS:O	1:A:950:ARG:HG2	2.16	0.46
1:B:338:VAL:HG22	1:B:543:SER:HB2	1.98	0.46
1:B:984:GLU:HG2	1:B:987:ILE:HD12	1.98	0.46
1:A:809:TRP:CZ2	1:A:938:LEU:HB2	2.51	0.46
1:B:468:MET:HE2	1:B:494:PHE:HD2	1.81	0.46
1:B:584:GLU:HB3	1:B:953:LYS:CE	2.33	0.46
1:B:1025:PRO:HG2	1:B:1027:PHE:CE1	2.51	0.46
1:A:260:LEU:HD22	1:A:264:GLU:CG	2.44	0.46
1:A:627:PHE:HA	1:A:958:PHE:HZ	1.81	0.46
1:A:810:THR:HA	1:B:1001:MET:CE	2.40	0.46
1:B:500:GLN:OE1	1:B:541:LEU:CB	2.46	0.46
1:B:770:HIS:HA	1:B:772:GLU:OE2	2.15	0.46
1:B:918:LYS:O	1:B:918:LYS:HG3	2.15	0.46
1:A:468:MET:HE2	1:A:494:PHE:HD2	1.81	0.46
1:A:585:ASN:HA	1:A:955:LEU:CD2	2.45	0.46
1:B:564:GLU:OE1	1:B:564:GLU:HA	2.16	0.46
1:B:933:TYR:HB3	1:B:971:ILE:HD11	1.98	0.46
1:A:627:PHE:HA	1:A:958:PHE:CZ	2.51	0.45
1:B:421:LYS:O	1:B:425:ILE:HG13	2.15	0.45
1:B:602:LYS:CE	1:B:948:LEU:CD1	2.86	0.45
1:B:926:CYS:C	1:B:928:PRO:HD3	2.40	0.45
1:A:583:GLU:HB3	1:A:950:ARG:CD	2.33	0.45
1:A:922:ILE:C	1:A:922:ILE:HD12	2.41	0.45
1:B:199:GLN:HB3	1:B:203:ASP:CB	2.43	0.45
1:B:496:MET:C	1:B:497:ARG:HG3	2.41	0.45
1:B:449:THR:CG2	1:B:458:GLU:OE1	2.61	0.45
1:B:221:LEU:CB	1:B:554:LEU:HD22	2.46	0.45
1:B:419:ILE:O	1:B:419:ILE:CG2	2.62	0.45
1:B:1043:SER:C	1:B:1045:PRO:HD3	2.41	0.45
1:A:552:ARG:O	1:A:553:MET:C	2.60	0.45
1:B:949:LYS:NZ	1:B:954:GLU:HB2	2.32	0.45
1:A:626:THR:HG22	1:A:958:PHE:CZ	2.52	0.45
1:A:927:VAL:O	1:A:928:PRO:C	2.59	0.45
1:A:1025:PRO:HG2	1:A:1027:PHE:CE1	2.51	0.45
1:B:470:CYS:HB2	1:B:492:GLU:HB2	1.99	0.45
1:B:731:GLU:OE1	1:B:731:GLU:HA	2.16	0.45
1:B:912:TYR:CZ	1:B:929:PHE:CE2	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:SER:HB3	1:A:370:LYS:HG3	1.99	0.45
1:A:634:PHE:CZ	1:A:958:PHE:CE1	3.05	0.45
1:B:298:TYR:CE2	1:B:302:ILE:HG13	2.52	0.45
1:B:364:SER:HB3	1:B:370:LYS:HG3	1.99	0.45
1:B:583:GLU:HG3	1:B:951:HIS:CD2	2.52	0.45
1:A:240:ASN:OD1	1:A:244:ASN:ND2	2.50	0.45
1:A:247:SER:OG	1:A:248:ARG:N	2.45	0.45
1:A:1043:SER:C	1:A:1045:PRO:HD3	2.41	0.45
1:A:506:ASP:C	1:A:508:ASN:H	2.25	0.44
1:B:471:CYS:HB3	1:B:488:TYR:HB3	2.00	0.44
1:A:470:CYS:HB2	1:A:492:GLU:HB2	1.99	0.44
1:B:506:ASP:C	1:B:508:ASN:H	2.25	0.44
1:B:945:PRO:HB3	1:B:947:VAL:O	2.17	0.44
1:A:601:ILE:N	1:A:601:ILE:HD12	2.32	0.44
1:B:602:LYS:HG2	1:B:948:LEU:HD12	1.99	0.44
1:B:603:ALA:HB1	1:B:955:LEU:HB2	1.99	0.44
1:B:603:ALA:HB1	1:B:955:LEU:HB3	1.99	0.44
1:A:298:TYR:CE2	1:A:302:ILE:HG13	2.52	0.44
1:B:371:GLU:O	1:B:375:GLN:HG2	2.18	0.44
1:B:603:ALA:HB1	1:B:955:LEU:C	2.42	0.44
1:B:224:LYS:HZ3	1:B:558:MET:HG2	1.83	0.44
1:A:292:PHE:HE2	1:A:353:TYR:CE2	2.36	0.44
1:A:341:ARG:HH22	1:A:536:ASN:N	2.16	0.44
1:A:999:ASN:ND2	1:B:938:LEU:HD11	2.33	0.44
1:B:248:ARG:HA	1:B:248:ARG:NE	2.33	0.43
1:B:422:MET:HG2	1:B:464:PHE:HE2	1.83	0.43
1:B:601:ILE:HD12	1:B:601:ILE:N	2.32	0.43
1:A:567:MET:HB2	1:A:568:ARG:H	1.54	0.43
1:B:292:PHE:HE2	1:B:353:TYR:CE2	2.36	0.43
1:A:471:CYS:HB3	1:A:488:TYR:HB3	1.99	0.43
1:A:654:GLU:CG	1:A:655:PRO:HD2	2.48	0.43
1:A:856:ILE:O	1:A:859:LEU:HB3	2.18	0.43
1:A:881:SER:OG	1:B:880:SER:C	2.61	0.43
1:B:237:PHE:HE1	1:B:314:GLN:HG3	1.83	0.43
1:B:558:MET:C	1:B:560:GLN:N	2.74	0.43
1:B:663:ILE:HG13	1:B:669:PRO:HG3	1.99	0.43
1:B:1022:LYS:HG3	1:B:1023:PRO:HD2	2.00	0.43
1:A:337:TYR:OH	1:A:502:ASN:CG	2.62	0.43
1:A:663:ILE:HG13	1:A:669:PRO:HG3	2.00	0.43
1:A:885:ARG:HB3	1:B:884:TYR:CE2	2.53	0.43
1:B:999:ASN:C	1:B:999:ASN:ND2	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:VAL:CG1	1:A:500:GLN:N	2.82	0.43
1:A:828:THR:HA	1:A:873:GLU:OE2	2.19	0.43
1:B:856:ILE:O	1:B:859:LEU:HB3	2.18	0.43
1:A:293:ASP:N	1:A:294:PRO:CD	2.82	0.43
1:A:422:MET:HG2	1:A:464:PHE:HE2	1.82	0.43
1:A:742:ILE:HG13	1:A:743:ALA:N	2.34	0.43
1:B:585:ASN:HA	1:B:955:LEU:HD11	2.00	0.43
1:A:339:LEU:N	1:A:340:PRO:HD2	2.34	0.43
1:B:459:ARG:HG2	1:B:459:ARG:NH1	2.32	0.43
1:B:499:VAL:CG1	1:B:500:GLN:N	2.82	0.43
1:B:742:ILE:HG13	1:B:743:ALA:N	2.34	0.43
1:A:1022:LYS:HG3	1:A:1023:PRO:HD2	2.01	0.43
1:A:605:THR:HG23	1:A:955:LEU:HD22	2.00	0.42
1:B:583:GLU:CG	1:B:951:HIS:HD2	2.31	0.42
1:B:824:MET:CE	1:B:930:PHE:CD2	3.02	0.42
1:B:872:LEU:HD23	1:B:872:LEU:H	1.81	0.42
1:A:590:GLU:CD	1:A:590:GLU:H	2.27	0.42
1:A:999:ASN:C	1:A:999:ASN:ND2	2.72	0.42
1:B:293:ASP:N	1:B:294:PRO:CD	2.82	0.42
1:B:201:TYR:CD2	1:B:364:SER:HA	2.55	0.42
1:B:422:MET:HG2	1:B:464:PHE:CE2	2.54	0.42
1:B:500:GLN:CD	1:B:541:LEU:HB3	2.37	0.42
1:B:630:THR:CG2	1:B:805:VAL:HG21	2.36	0.42
1:A:199:GLN:O	1:A:363:LYS:NZ	2.47	0.42
1:A:634:PHE:HE2	1:A:958:PHE:CE1	2.38	0.42
1:A:810:THR:CA	1:B:1001:MET:HE3	2.42	0.42
1:B:341:ARG:HH22	1:B:535:ASN:C	2.27	0.42
1:B:912:TYR:CZ	1:B:929:PHE:HE2	2.38	0.42
1:A:269:MET:HE1	1:A:729:TRP:HD1	1.84	0.42
1:A:702:TYR:O	1:A:706:ARG:HG3	2.19	0.42
1:B:339:LEU:N	1:B:340:PRO:HD2	2.34	0.42
1:A:325:GLN:HG3	1:A:332:LYS:HD2	2.02	0.42
1:A:422:MET:HE1	1:A:438:GLY:HA2	2.02	0.42
1:A:459:ARG:HG2	1:A:459:ARG:NH1	2.32	0.42
1:A:950:ARG:C	1:A:952:GLY:N	2.77	0.42
1:B:582:SER:H	1:B:585:ASN:ND2	2.16	0.42
1:B:702:TYR:O	1:B:706:ARG:HG3	2.19	0.42
1:B:828:THR:HA	1:B:873:GLU:OE2	2.19	0.42
1:B:922:ILE:HD12	1:B:922:ILE:C	2.45	0.42
1:A:958:PHE:CD2	1:A:962:ARG:HG3	2.55	0.42
1:B:208:PHE:CE1	1:B:353:TYR:HE1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:MET:HE1	1:B:438:GLY:HA2	2.02	0.42
1:B:796:TYR:CZ	1:B:971:ILE:HG23	2.52	0.42
1:A:217:ARG:NH1	1:A:554:LEU:HD23	2.35	0.41
1:A:226:PHE:HZ	1:A:550:LEU:CD1	2.31	0.41
1:A:422:MET:HG2	1:A:464:PHE:CE2	2.54	0.41
1:A:587:ILE:HD12	1:A:603:ALA:C	2.45	0.41
1:B:325:GLN:HG3	1:B:332:LYS:HD2	2.02	0.41
1:B:338:VAL:CG2	1:B:543:SER:HB2	2.50	0.41
1:B:564:GLU:HB2	1:B:676:ARG:HH12	1.82	0.41
1:B:901:LEU:HD11	1:B:905:HIS:CE1	2.55	0.41
1:A:208:PHE:CE1	1:A:353:TYR:HE1	2.37	0.41
1:A:295:TYR:CD1	1:A:350:CYS:HB2	2.55	0.41
1:A:630:THR:CG2	1:A:965:ALA:CB	2.97	0.41
1:A:402:GLU:HA	1:A:402:GLU:OE1	2.19	0.41
1:B:583:GLU:HG3	1:B:951:HIS:HD2	1.86	0.41
1:A:583:GLU:C	1:A:950:ARG:HB3	2.44	0.41
1:A:459:ARG:NE	1:A:492:GLU:OE1	2.54	0.41
1:A:567:MET:O	1:A:568:ARG:CB	2.69	0.41
1:B:668:GLN:HA	1:B:669:PRO:HD3	1.82	0.41
1:A:304:ARG:HA	1:A:305:PRO:HD3	1.98	0.41
1:A:371:GLU:HA	1:A:371:GLU:OE1	2.21	0.41
1:B:269:MET:O	1:B:269:MET:HG2	2.21	0.41
1:B:295:TYR:CD1	1:B:350:CYS:HB2	2.55	0.41
1:B:428:ASN:C	1:B:486:ALA:HB1	2.45	0.41
1:B:893:ILE:O	1:B:898:LYS:HE3	2.20	0.41
1:A:570:PRO:HD2	1:A:677:PHE:CZ	2.56	0.41
1:B:687:LEU:HG	1:B:726:MET:HE1	2.03	0.41
1:A:474:ASN:HB2	1:A:479:ARG:NH2	2.36	0.41
1:A:586:ILE:HA	1:A:604:GLY:HA2	2.03	0.41
1:A:508:ASN:C	1:A:510:TYR:H	2.29	0.40
1:A:731:GLU:HG2	1:A:735:LYS:HE3	2.02	0.40
1:A:893:ILE:O	1:A:898:LYS:HE3	2.20	0.40
1:B:508:ASN:C	1:B:510:TYR:H	2.29	0.40
1:B:953:LYS:HD3	1:B:953:LYS:HA	1.94	0.40
1:A:587:ILE:CD1	1:A:603:ALA:C	2.95	0.40
1:A:687:LEU:HG	1:A:726:MET:HE1	2.03	0.40
1:B:456:LYS:H	1:B:456:LYS:HG2	1.62	0.40
1:B:459:ARG:NE	1:B:492:GLU:OE1	2.54	0.40
1:A:217:ARG:HH21	1:A:551:GLU:HG2	1.85	0.40
1:A:457:HIS:CD2	1:A:472:LYS:NZ	2.90	0.40
1:A:479:ARG:HG2	1:A:479:ARG:NH1	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:LEU:HD11	1:A:934:LEU:HD21	2.02	0.40
1:B:221:LEU:HD12	1:B:554:LEU:HB2	2.03	0.40
1:B:371:GLU:HA	1:B:371:GLU:OE1	2.21	0.40
1:B:961:ARG:H	1:B:961:ARG:HD2	1.86	0.40
1:A:901:LEU:O	1:A:905:HIS:ND1	2.51	0.40
1:B:604:GLY:CA	1:B:955:LEU:HD12	2.37	0.40
1:A:212:ILE:CG2	1:A:260:LEU:HG	2.51	0.40
1:B:419:ILE:CG2	1:B:422:MET:HB2	2.52	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:PRO:CB	1:B:753:THR:OG1[4_555]	1.85	0.35
1:A:392:SER:CB	1:A:507:THR:CG2[4_556]	2.00	0.20

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	816/852 (96%)	774 (95%)	36 (4%)	6 (1%)	18	48
1	B	816/852 (96%)	775 (95%)	34 (4%)	7 (1%)	14	43
All	All	1632/1704 (96%)	1549 (95%)	70 (4%)	13 (1%)	16	45

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	567	MET
1	A	1045	PRO
1	B	1045	PRO
1	A	497	ARG

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Mol	Chain	Res	Type
1	A	508	ASN
1	A	568	ARG
1	B	497	ARG
1	B	508	ASN
1	A	440	CYS
1	B	440	CYS
1	B	565	GLU
1	B	959	SER
1	B	924	PRO

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	754/777 (97%)	722 (96%)	32 (4%)	26	49
1	B	754/777 (97%)	729 (97%)	25 (3%)	33	54
All	All	1508/1554 (97%)	1451 (96%)	57 (4%)	29	51

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	GLN
1	A	255	LEU
1	A	258	LYS
1	A	259	LEU
1	A	260	LEU
1	A	310	ARG
1	A	356	LEU
1	A	439	GLN
1	A	458	GLU
1	A	463	LEU
1	A	498	LYS
1	A	500	GLN
1	A	544	LEU
1	A	556	VAL

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Mol	Chain	Res	Type
1	A	560	GLN
1	A	567	MET
1	A	570	PRO
1	A	580	PRO
1	A	585	ASN
1	A	587	ILE
1	A	609	LEU
1	A	640	LEU
1	A	647	ARG
1	A	772	GLU
1	A	804	LEU
1	A	830	ASN
1	A	928	PRO
1	A	955	LEU
1	A	966	GLU
1	A	989	ARG
1	A	999	ASN
1	A	1003	LYS
1	B	214	GLN
1	B	255	LEU
1	B	258	LYS
1	B	259	LEU
1	B	260	LEU
1	B	356	LEU
1	B	439	GLN
1	B	458	GLU
1	B	463	LEU
1	B	498	LYS
1	B	544	LEU
1	B	585	ASN
1	B	609	LEU
1	B	640	LEU
1	B	647	ARG
1	B	772	GLU
1	B	804	LEU
1	B	830	ASN
1	B	872	LEU
1	B	945	PRO
1	B	966	GLU
1	B	989	ARG
1	B	999	ASN
1	B	1003	LYS

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Mol	Chain	Res	Type
1	B	1045	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	GLN
1	A	244	ASN
1	A	276	HIS
1	A	352	HIS
1	A	359	GLN
1	A	375	GLN
1	A	428	ASN
1	A	457	HIS
1	A	475	HIS
1	A	477	GLN
1	A	502	ASN
1	A	508	ASN
1	A	545	GLN
1	A	585	ASN
1	A	695	HIS
1	A	699	HIS
1	A	712	GLN
1	A	755	GLN
1	A	770	HIS
1	A	860	GLN
1	A	879	ASN
1	A	905	HIS
1	A	911	HIS
1	A	923	ASN
1	A	972	GLN
1	A	999	ASN
1	B	240	ASN
1	B	244	ASN
1	B	276	HIS
1	B	352	HIS
1	B	359	GLN
1	B	428	ASN
1	B	457	HIS
1	B	475	HIS
1	B	477	GLN
1	B	585	ASN
1	B	691	ASN

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Mol	Chain	Res	Type
1	B	695	HIS
1	B	738	GLN
1	B	860	GLN
1	B	905	HIS
1	B	923	ASN
1	B	936	ASN
1	B	951	HIS
1	B	972	GLN
1	B	999	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	824/852 (96%)	-0.35	1 (0%)	92 86	35, 135, 288, 306	0
1	B	824/852 (96%)	-0.29	1 (0%)	92 86	29, 143, 289, 306	0
All	All	1648/1704 (96%)	-0.32	2 (0%)	92 86	29, 139, 289, 306	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	271	ASP	3.0
1	A	958	PHE	2.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.