



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:28 PM GMT

PDB ID : 1XD4
Title : Crystal structure of the DH-PH-cat module of Son of Sevenless (SOS)
Authors : Sondermann, H.; Soisson, S.M.; Boykevisch, 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
<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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

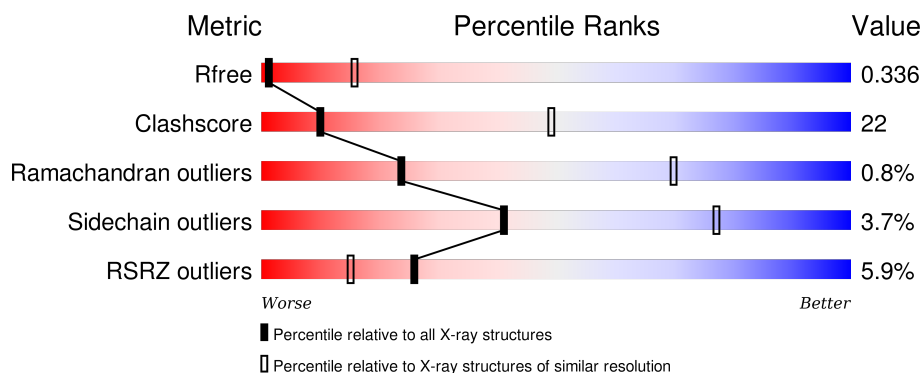
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1014 (3.80-3.48)
Clashscore	102246	1130 (3.80-3.48)
Ramachandran outliers	100387	1084 (3.80-3.48)
Sidechain outliers	100360	1083 (3.80-3.48)
RSRZ outliers	91569	1021 (3.80-3.48)

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	852	<div> <div>5%</div> <div>67%</div> <div>27%</div> <div>• •</div> </div>
1	B	852	<div> <div>6%</div> <div>67%</div> <div>28%</div> <div>• •</div> </div>

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.

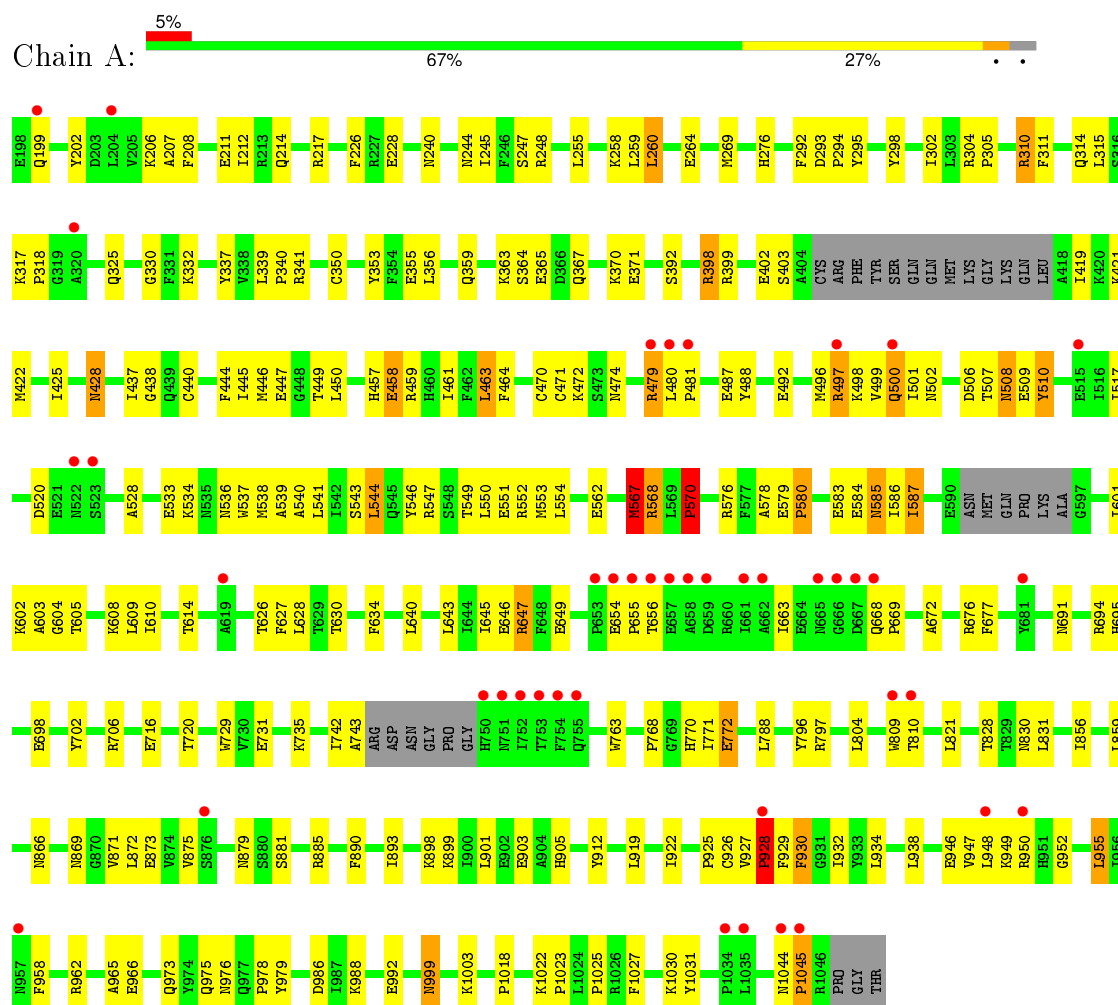
- Molecule 1 is a protein called Son of sevenless protein homolog 1.

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			

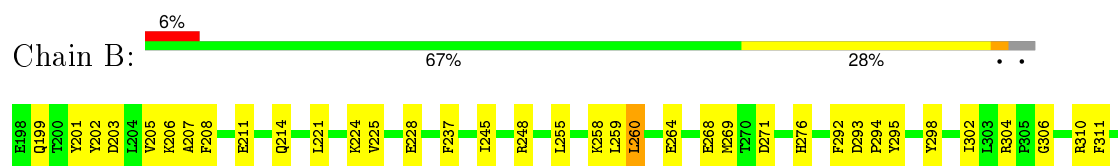
3 Residue-property plots

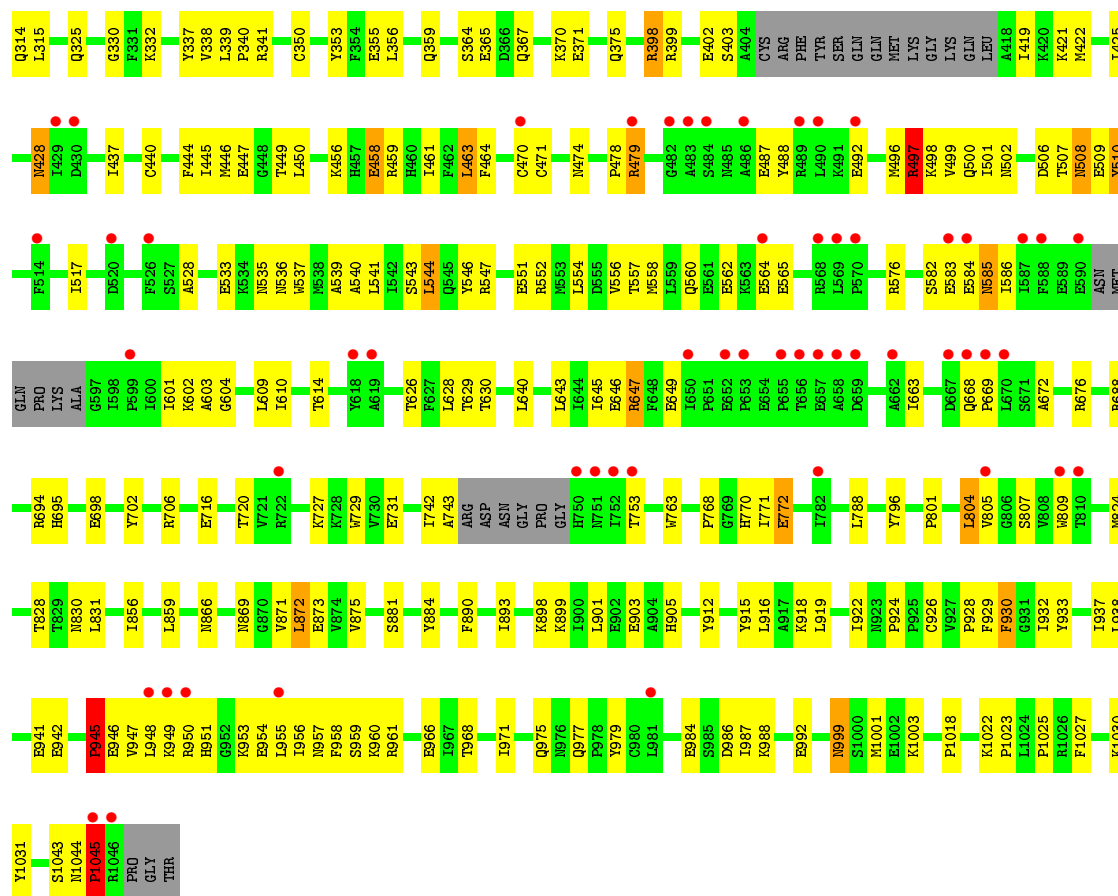
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: Son of sevenless protein homolog 1



- Molecule 1: Son of sevenless protein homolog 1





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 47.02 – 3.64	Depositor EDS
% Data completeness (in resolution range)	92.0 (11.99-3.64) 92.1 (47.02-3.64)	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 (7.55%)	DCC
Wilson B-factor (Å ²)	131.1	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 149.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 29443 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.90	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.47	0/6918	0.69	5/9334 (0.1%)
1	B	0.47	0/6918	0.68	3/9334 (0.0%)
All	All	0.47	0/13836	0.68	8/18668 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	945	PRO	CA-N-CD	-16.27	88.72	111.50
1	A	580	PRO	CA-N-CD	-16.02	89.06	111.50
1	A	928	PRO	CA-N-CD	-14.33	91.44	111.50
1	A	570	PRO	CA-N-CD	-9.07	98.81	111.50
1	A	310	ARG	NE-CZ-NH2	6.49	123.54	120.30
1	B	398	ARG	NE-CZ-NH2	6.49	123.54	120.30
1	A	398	ARG	NE-CZ-NH2	6.33	123.46	120.30
1	B	497	ARG	NE-CZ-NH2	5.59	123.10	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	6771	0	6768	293	1
1	B	6771	0	6768	309	1
All	All	13542	0	13536	596	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 22.

All (596) 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
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:B:422:MET:HE3	1:B:437:ILE:HG22	1.48	0.96
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:A:317:LYS:HG2	1:A:318:PRO:HD2	1.48	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:A:422:MET:HE3	1:A:437:ILE:HG22	1.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:875:VAL:HG13	1:B:905:HIS:HD2	1.38	0.88
1:A:716:GLU:O	1:A:720:THR:HG23	1.72	0.88
1:B:602:LYS:HE2	1:B:948:LEU:CD1	2.04	0.87
1:A:919:LEU:HD11	1:A:928:PRO:HG3	1.56	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:CD1	1:A:928:PRO:HG3	2.05	0.87
1:B:584:GLU:HA	1:B:953:LYS:CB	2.04	0.86
1:B:269:MET:SD	1:B:729:TRP:CD1	2.68	0.86
1:B:630:THR:HG22	1:B:805:VAL:CG2	2.05	0.86
1:A:428:ASN:ND2	1:A:487:GLU:H	1.72	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:HG22	1:A:958:PHE:HE2	1.41	0.82
1:A:626:THR:CG2	1:A:962:ARG:CG	2.56	0.82
1:B:629:THR:HG23	1:B:801:PRO:HB2	1.62	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:A:587:ILE:N	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
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:B:584:GLU:CB	1:B:953:LYS:CD	2.62	0.76
1:A:500:GLN:NE2	1:A:538:MET:SD	2.58	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:B:446:MET:HE1	1:B:537:TRP:HA	1.67	0.76
1:B:499:VAL:CG1	1:B:501:ILE:CD1	2.63	0.76
1:A:628:LEU:HD12	1:A:695:HIS:CD2	2.20	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: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:O	1:A:520:ASP:OD1	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:B:584:GLU:CA	1:B:953:LYS:CG	2.44	0.74
1:A:926:CYS:SG	1:A:928:PRO:HD2	2.28	0.74
1:A:831:LEU:HD23	1:A:873:GLU:OE1	1.87	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:A:202:TYR:CE2	1:A:206:LYS:HD3	2.22	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:A:446:MET:HE1	1:A:537:TRP:HA	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:901:LEU:CG	1:A:905:HIS:HE1	2.03	0.70
1:A:614:THR:OG1	1:A:647:ARG:HD3	1.90	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:199:GLN:HB3	1:B:203:ASP:HB2	1.72	0.70
1:B:422:MET:CE	1:B:437:ILE:HG22	2.20	0.70
1:B:809:TRP:HH2	1:B:937:ILE:HG22	1.55	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: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:O	1:A:419:ILE:HG22	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:958:PHE:CE2	1:A:962:ARG:HG2	2.28	0.69
1:A:330:GLY:CA	1:A:546:TYR:CE2	2.75	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: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:587:ILE:HD13	1:A:603:ALA:HB3	0.81	0.68
1:A:539:ALA:O	1:A:543:SER:HB2	1.94	0.68
1:A:276:HIS:HE1	1:A:365:GLU:H	1.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:498:LYS:HD2	1:B:517:ILE:O	1.95	0.67
1:A:881:SER:N	1:B:881:SER:OG	2.28	0.67
1:B:341:ARG:HG3	1:B:403:SER:OG	1.95	0.66
1:B:947:VAL:HB	1:B:955:LEU:O	1.94	0.66
1:A:226:PHE:HZ	1:A:550:LEU:HD13	1.61	0.66
1:B:445:ILE:HD13	1:B:544:LEU:HD23	1.78	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:901:LEU:CG	1:A:905:HIS:CE1	2.78	0.66
1:A:498:LYS:HD2	1:A:517:ILE:O	1.95	0.66
1:A:507:THR:C	1:A:509:GLU:H	1.99	0.66
1:B:630:THR:CA	1:B:805:VAL:HG11	2.26	0.65
1:B:507:THR:C	1:B:509:GLU:H	1.99	0.65
1:B:237:PHE:HD1	1:B:314:GLN:OE1	1.78	0.65
1:B:872:LEU:CD2	1:B:872:LEU:N	2.60	0.65
1:A:269:MET:SD	1:A:729:TRP:CD1	2.89	0.65
1:B:926:CYS:O	1:B:928:PRO:HD3	1.96	0.65
1:A:1044:ASN:N	1:A:1045:PRO:HD3	2.12	0.65
1:B:901:LEU:CD1	1:B:905:HIS:NE2	2.60	0.65
1:A:444:PHE:HZ	1:A:447:GLU:HB2	1.62	0.65
1:B:872:LEU:HD23	1:B:872:LEU:N	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:A:502:ASN:HD21	1:A:534:LYS:HZ3	1.46	0.64
1:B:1044:ASN:N	1:B:1045:PRO:HD3	2.12	0.64
1:B:796:TYR:CE2	1:B:975:GLN:HG3	2.31	0.64
1:B:584:GLU:HA	1:B:953:LYS:HB3	1.80	0.64
1:A:226:PHE:CZ	1:A:550:LEU:HD13	2.33	0.64
1:A:586:ILE:HD11	1:A:601:ILE:HG13	1.78	0.64
1:A:496:MET:C	1:A:497:ARG:HG3	2.17	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:HG2	1:B:459:ARG:HH11	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:B:901:LEU:HG	1:B:905:HIS:HE1	1.53	0.63
1:A:499:VAL:CG1	1:A:501:ILE:HD11	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:LEU:CD1	1:A:481:PRO:HD2	2.27	0.63
1:B:341:ARG:HH12	1:B:535:ASN:HB3	1.63	0.63
1:A:919:LEU:HD13	1:A:928:PRO:HG3	1.81	0.63
1:A:459:ARG:HG2	1:A:459:ARG:HH11	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:B:584:GLU:HB3	1:B:953:LYS:HG3	1.79	0.62
1:B:499:VAL:CG1	1:B:501:ILE:HD11	2.28	0.62
1:A:788:LEU:HD13	1:A:831:LEU:HD21	1.81	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:269:MET:SD	1:B:729:TRP:NE1	2.72	0.62
1:B:224:LYS:HB3	1:B:557:THR:HG21	1.82	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:HA	1:B:1003:LYS:HE3	1.82	0.62
1:B:999:ASN:C	1:B:999:ASN:HD22	2.02	0.62
1:B:630:THR:CB	1:B:805:VAL:HG11	2.29	0.62
1:B:954:GLU:C	1:B:955:LEU:HD22	2.20	0.61
1:A:317:LYS:HG3	1:A:318:PRO:CD	2.29	0.61
1:A:446:MET:HE3	1:A:537:TRP:CE3	2.34	0.61
1:B:496:MET:O	1:B:497:ARG:CG	2.48	0.61
1:A:999:ASN:HD22	1:A:999:ASN:C	2.02	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:450:LEU:HD12	1:A:461:ILE:HD12	1.83	0.61
1:B:450:LEU:HD12	1:B:461:ILE:HD12	1.83	0.61
1:A:672:ALA:O	1:A:676:ARG:HG3	2.00	0.61
1:A:364:SER:HB3	1:A:370:LYS:HG2	1.83	0.61
1:B:585:ASN:C	1:B:955:LEU:HD11	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:645:ILE:O	1:B:649:GLU:HG2	2.01	0.60
1:A:1003:LYS:HA	1:A:1003:LYS:HE3	1.82	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:A:260:LEU:HD22	1:A:264:GLU:HG3	1.83	0.60
1:B:260:LEU:HD22	1:B:264:GLU:HG3	1.83	0.60
1:A:587:ILE:O	1:A:602:LYS:N	2.33	0.60
1:A:337:TYR:CD2	1:A:538:MET:CB	2.84	0.60
1:B:202:TYR:O	1:B:206:LYS:HG3	2.01	0.60
1:A:796:TYR:HD1	1:A:930:PHE:HD2	1.49	0.60
1:B:539:ALA:O	1:B:543:SER:HB3	2.01	0.60
1:B:584:GLU:OE1	1:B:953:LYS:HE3	2.02	0.60
1:B:364:SER:HB3	1:B:370:LYS:CG	2.31	0.60
1:B:564:GLU:HB2	1:B:676:ARG:NH1	2.16	0.60
1:A:364:SER:HB3	1:A:370:LYS:CG	2.32	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:B:330:GLY:HA2	1:B:546:TYR:CE2	2.37	0.59
1:A:539:ALA:O	1:A:543:SER:CB	2.50	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: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: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: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:260:LEU:O	1:A:264:GLU:HG3	2.03	0.58
1:A:587:ILE:HD12	1:A:587:ILE:H	1.67	0.58
1:B:926:CYS:HA	1:B:979:TYR:OH	2.03	0.58
1:B:498:LYS:HB3	1:B:517:ILE:O	2.04	0.58
1:B:445:ILE:CD1	1:B:544:LEU:CD2	2.81	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:TYR:CD2	1:A:538:MET:HB3	2.38	0.58
1:B:901:LEU:CD1	1:B:905:HIS:CE1	2.86	0.58
1:B:630:THR:HA	1:B:805:VAL:HG11	1.86	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:890:PHE:O	1:A:898:LYS:HE2	2.04	0.57
1:A:950:ARG:HB2	1:A:955:LEU:HD11	1.87	0.57
1:A:498:LYS:HB3	1:A:517:ILE:O	2.04	0.57
1:A:537:TRP:O	1:A:541:LEU:HG	2.03	0.57
1:B:341:ARG:NH2	1:B:536:ASN:N	2.51	0.57
1:B:446:MET:HE3	1:B:537:TRP:CE3	2.40	0.57
1:A:796:TYR:CE1	1:A:930:PHE:CD2	2.92	0.57
1:B:875:VAL:CG1	1:B:905:HIS:HD2	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:629:THR:HG23	1:B:801:PRO:HB3	1.86	0.55
1:B:626:THR:CG2	1:B:958:PHE:CZ	2.89	0.55
1:B:276:HIS:CE1	1:B:365:GLU:H	2.22	0.55
1:A:479:ARG:HH11	1:A:479:ARG:HG2	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:B:915:TYR:OH	1:B:929:PHE:N	2.39	0.55
1:A:498:LYS:HD3	1:A:499:VAL:H	1.71	0.55
1:B:224:LYS:NZ	1:B:558:MET:HG2	2.22	0.55
1:B:201:TYR:O	1:B:205:VAL:HG23	2.07	0.55
1:B:582:SER:H	1:B:585:ASN:HD21	1.54	0.54
1:A:694:ARG:O	1:A:698:GLU:HB2	2.07	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:O	1:A:544:LEU:HD13	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:B:604:GLY:O	1:B:956:ILE:HG12	2.08	0.54
1:A:585:ASN:OD1	1:A:608:LYS:HE3	2.08	0.54
1:A:507:THR:O	1:A:509:GLU:N	2.40	0.53
1:B:560:GLN:C	1:B:562:GLU:H	2.10	0.53
1:B:809:TRP:CH2	1:B:937:ILE:HG22	2.41	0.53
1:B:727:LYS:O	1:B:731:GLU:HG2	2.09	0.53
1:A:587:ILE:N	1:A:603:ALA:O	2.34	0.53
1:B:544:LEU:HD13	1:B:544:LEU:O	2.10	0.52
1:B:958:PHE:C	1:B:960:LYS:H	2.12	0.52
1:B:915:TYR:OH	1:B:929:PHE:HB3	2.08	0.52
1:B:912:TYR:CE1	1:B:929:PHE:CE2	2.98	0.52
1:A:269:MET:HG3	1:A:691:ASN:OD1	2.10	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:B:933:TYR:O	1:B:937:ILE:HG13	2.10	0.51
1:B:221:LEU:CD1	1:B:554:LEU:HD22	2.40	0.51
1:A:810:THR:HB	1:B:999:ASN:O	2.09	0.51
1:B:796:TYR:HE2	1:B:975:GLN:HG3	1.73	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:630:THR:CG2	1:A:965:ALA:HB2	2.40	0.51
1:A:474:ASN:HB2	1:A:479:ARG:HH21	1.75	0.51
1:B:610:ILE:HD12	1:B:643:LEU:HD13	1.93	0.51
1:B:311:PHE:O	1:B:315:LEU:HD13	2.10	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:A:499:VAL:HG12	1:A:500:GLN:N	2.26	0.51
1:B:552:ARG:O	1:B:556:VAL:HG23	2.11	0.51
1:A:810:THR:HA	1:B:1001:MET:CE	2.40	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
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: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:568:ARG:HH12	1:A:656:THR:HG22	1.77	0.50
1:B:763:TRP:CE2	1:B:768:PRO:HG3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:500:GLN:NE2	1:A:538:MET:HE1	2.25	0.50
1:A:480:LEU:CG	1:A:481:PRO:HD2	2.41	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:955:LEU:N	1:B:955:LEU:HD22	2.27	0.50
1:B:628:LEU:CD1	1:B:695:HIS:HD2	2.15	0.50
1:A:500:GLN:HE22	1:A:538:MET:HE3	1.75	0.50
1:B:474:ASN:HB2	1:B:479:ARG:HH21	1.75	0.50
1:A:445:ILE:HD11	1:A:544:LEU:CD2	2.42	0.49
1:B:539:ALA:O	1:B:543:SER:CB	2.61	0.49
1:B:977:GLN:OE1	1:B:977:GLN:N	2.44	0.49
1:B:446:MET:CE	1:B:463:LEU:HD12	2.43	0.49
1:A:446:MET:CE	1:A:463:LEU:HD12	2.42	0.49
1:B:399:ARG:O	1:B:402:GLU:HB2	2.13	0.49
1:A:771:ILE:HG22	1:A:986:ASP:HB3	1.95	0.49
1:B:306:GLY:O	1:B:310:ARG:HD2	2.13	0.49
1:A:480:LEU:HG	1:A:481:PRO:HD2	1.95	0.49
1:A:269:MET:CE	1:A:729:TRP:HD1	2.25	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: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:866:ASN:HB3	1:A:926:CYS:CB	2.43	0.48
1:A:796:TYR:CE1	1:A:930:PHE:CE2	3.01	0.48
1:B:603:ALA:CB	1:B:955:LEU:HB2	2.44	0.48
1:A:337:TYR:CD2	1:A:538:MET:HB2	2.48	0.48
1:A:502:ASN:ND2	1:A:534:LYS:NZ	2.59	0.48
1:A:587:ILE:HD12	1:A:603:ALA:O	2.14	0.48
1:B:630:THR:HG22	1:B:805:VAL:HG22	1.92	0.48
1:A:1030:LYS:HD2	1:A:1031:TYR:CZ	2.48	0.48
1:A:217:ARG:HH12	1:A:554:LEU:HD23	1.79	0.48
1:A:446:MET:HE2	1:A:463:LEU:HD12	1.96	0.48
1:B:474:ASN:CB	1:B:479:ARG:HH21	2.27	0.48
1:B:875:VAL:HG22	1:B:905:HIS:CD2	2.49	0.48
1:A:568:ARG:NH1	1:A:656:THR:HG22	2.29	0.48
1:A:449:THR:CG2	1:A:458:GLU:OE1	2.61	0.48
1:A:587:ILE:HG13	1:A:950:ARG:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:LEU:HD22	1:B:264:GLU:CG	2.44	0.47
1:A:950:ARG:C	1:A:952:GLY:H	2.17	0.47
1:B:507:THR:C	1:B:509:GLU:N	2.67	0.47
1:A:634:PHE:CZ	1:A:958:PHE:HD1	2.31	0.47
1:A:399:ARG:O	1:A:402:GLU:HB2	2.14	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:341:ARG:NH2	1:A:536:ASN:OD1	2.47	0.47
1:A:245:ILE:HD11	1:A:314:GLN:HG2	1.96	0.47
1:B:603:ALA:CB	1:B:955:LEU:CB	2.92	0.47
1:B:947:VAL:CB	1:B:955:LEU:O	2.60	0.47
1:B:500:GLN:C	1:B:501:ILE:HD12	2.35	0.47
1:A:445:ILE:CD1	1:A:544:LEU:CD2	2.92	0.47
1:A:446:MET:CE	1:A:540:ALA:HB3	2.45	0.47
1:B:922:ILE:O	1:B:922:ILE:HD12	2.13	0.47
1:A:654:GLU:HG2	1:A:655:PRO:HD2	1.95	0.47
1:B:585:ASN:C	1:B:955:LEU:CD1	2.83	0.47
1:B:458:GLU:HG3	1:B:458:GLU:O	2.13	0.47
1:A:458:GLU:HG3	1:A:458:GLU:O	2.14	0.47
1:A:567:MET:SD	1:A:567:MET:N	2.87	0.47
1:A:528:ALA:HB1	1:A:533:GLU:HB3	1.97	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:228:GLU:HA	1:A:228:GLU:OE1	2.15	0.47
1:A:668:GLN:HA	1:A:669:PRO:HD3	1.82	0.47
1:B:228:GLU:OE1	1:B:228:GLU:HA	2.15	0.47
1:A:500:GLN:C	1:A:501:ILE:HD12	2.35	0.46
1:A:421:LYS:O	1:A:425:ILE:HG13	2.15	0.46
1:B:603:ALA:C	1:B:955:LEU:HB3	2.35	0.46
1:A:217:ARG:HG3	1:A:217:ARG:HH11	1.80	0.46
1:B:629:THR:CG2	1:B:801:PRO:HB3	2.45	0.46
1:A:506:ASP:C	1:A:508:ASN:N	2.68	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:824:MET:HE3	1:B:930:PHE:CD2	2.51	0.46
1:B:510:TYR:CD1	1:B:510:TYR:O	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:A:510:TYR:CD1	1:A:510:TYR:O	2.69	0.46
1:B:984:GLU:HG2	1:B:987:ILE:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:ASP:C	1:B:508:ASN:N	2.68	0.46
1:A:809:TRP:CZ2	1:A:938:LEU:HB2	2.51	0.46
1:B:584:GLU:HB3	1:B:953:LYS:CE	2.33	0.46
1:B:585:ASN:C	1:B:585:ASN:HD22	2.19	0.46
1:B:1025:PRO:HG2	1:B:1027:PHE:CE1	2.51	0.46
1:B:918:LYS:HG3	1:B:918:LYS:O	2.15	0.46
1:A:627:PHE:HA	1:A:958:PHE:HZ	1.81	0.46
1:B:500:GLN:OE1	1:B:541:LEU:CB	2.46	0.46
1:A:260:LEU:HD22	1:A:264:GLU:CG	2.44	0.46
1:B:770:HIS:HA	1:B:772:GLU:OE2	2.15	0.46
1:A:585:ASN:HA	1:A:955:LEU:CD2	2.45	0.46
1:B:933:TYR:HB3	1:B:971:ILE:HD11	1.98	0.46
1:B:564:GLU:OE1	1:B:564:GLU:HA	2.16	0.46
1:A:627:PHE:HA	1:A:958:PHE:CZ	2.51	0.45
1:B:602:LYS:CE	1:B:948:LEU:CD1	2.86	0.45
1:B:421:LYS:O	1:B:425:ILE:HG13	2.15	0.45
1:A:583:GLU:HB3	1:A:950:ARG:CD	2.33	0.45
1:B:199:GLN:HB3	1:B:203:ASP:CB	2.43	0.45
1:A:446:MET:HE2	1:A:540:ALA:HB3	1.97	0.45
1:B:449:THR:CG2	1:B:458:GLU:OE1	2.61	0.45
1:B:419:ILE:CG2	1:B:419:ILE:O	2.62	0.45
1:B:221:LEU:CB	1:B:554:LEU:HD22	2.46	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:B:912:TYR:CZ	1:B:929:PHE:CE2	3.05	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:A:1025:PRO:HG2	1:A:1027:PHE:CE1	2.51	0.45
1:A:634:PHE:CZ	1:A:958:PHE:CE1	3.05	0.45
1:A:364:SER:HB3	1:A:370:LYS:HG3	1.99	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:B:298:TYR:CE2	1:B:302:ILE:HG13	2.52	0.45
1:A:507:THR:C	1:A:509:GLU:N	2.68	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:B:471:CYS:HB3	1:B:488:TYR:HB3	2.00	0.44
1:B:945:PRO:HB3	1:B:947:VAL:O	2.17	0.44
1:A:470:CYS:HB2	1:A:492:GLU:HB2	1.99	0.44
1:A:601:ILE:N	1:A:601:ILE:HD12	2.32	0.44
1:B:603:ALA:HB1	1:B:955:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:ALA:HB1	1:B:955:LEU:HB3	1.99	0.44
1:B:602:LYS:HG2	1:B:948:LEU:HD12	1.99	0.44
1:B:558:MET:C	1:B:560:GLN:H	2.21	0.44
1:B:371:GLU:O	1:B:375:GLN:HG2	2.18	0.44
1:A:298:TYR:CE2	1:A:302:ILE:HG13	2.52	0.44
1:B:224:LYS:HZ3	1:B:558:MET:HG2	1.83	0.44
1:A:578:ALA:O	1:A:579:GLU:C	2.54	0.44
1:A:341:ARG:HH22	1:A:536:ASN:N	2.16	0.44
1:A:292:PHE:HE2	1:A:353:TYR:CE2	2.36	0.44
1:B:958:PHE:C	1:B:960:LYS:N	2.71	0.44
1:A:999:ASN:ND2	1:B:938:LEU:HD11	2.33	0.44
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:B:248:ARG:NE	1:B:248:ARG:HA	2.33	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:422:MET:HE1	1:A:438:GLY:HA2	2.00	0.43
1:A:856:ILE:O	1:A:859:LEU:HB3	2.18	0.43
1:B:237:PHE:HE1	1:B:314:GLN:HG3	1.83	0.43
1:A:654:GLU:CG	1:A:655:PRO:HD2	2.48	0.43
1:A:471:CYS:HB3	1:A:488:TYR:HB3	1.99	0.43
1:B:1022:LYS:HG3	1:B:1023:PRO:HD2	2.00	0.43
1:B:663:ILE:HG13	1:B:669:PRO:HG3	1.99	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: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:B:585:ASN:HA	1:B:955:LEU:HD11	2.00	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:499:VAL:CG1	1:B:500:GLN:N	2.82	0.43
1:B:459:ARG:NH1	1:B:459:ARG:HG2	2.32	0.43
1:B:742:ILE:HG13	1:B:743:ALA:N	2.34	0.43
1:A:339:LEU:N	1:A:340:PRO:HD2	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:872:LEU:HD23	1:B:872:LEU:H	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:MET:HE2	1:A:729:TRP:HD1	1.85	0.42
1:B:999:ASN:C	1:B:999:ASN:ND2	2.72	0.42
1:B:293:ASP:N	1:B:294:PRO:CD	2.82	0.42
1:B:422:MET:HG2	1:B:464:PHE:CE2	2.54	0.42
1:B:201:TYR:CD2	1:B:364:SER:HA	2.55	0.42
1:B:630:THR:CG2	1:B:805:VAL:HG21	2.36	0.42
1:A:634:PHE:HE2	1:A:958:PHE:CE1	2.38	0.42
1:B:912:TYR:CZ	1:B:929:PHE:HE2	2.38	0.42
1:A:199:GLN:O	1:A:363:LYS:NZ	2.47	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:B:582:SER:H	1:B:585:ASN:ND2	2.16	0.42
1:A:459:ARG:HG2	1:A:459:ARG:NH1	2.32	0.42
1:A:325:GLN:HG3	1:A:332:LYS:HD2	2.02	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:446:MET:HE2	1:B:463:LEU:HD12	2.01	0.42
1:B:560:GLN:C	1:B:562:GLU:N	2.74	0.42
1:A:958:PHE:CD2	1:A:962:ARG:HG3	2.55	0.42
1:B:796:TYR:CZ	1:B:971:ILE:HG23	2.52	0.42
1:B:208:PHE:CE1	1:B:353:TYR:HE1	2.37	0.42
1:A:226:PHE:HZ	1:A:550:LEU:CD1	2.31	0.41
1:A:217:ARG:NH1	1:A:554:LEU:HD23	2.35	0.41
1:B:901:LEU:HD11	1:B:905:HIS:CE1	2.55	0.41
1:A:422:MET:HG2	1:A:464:PHE:CE2	2.54	0.41
1:B:564:GLU:HB2	1:B:676:ARG:HH12	1.82	0.41
1:B:338:VAL:CG2	1:B:543:SER:HB2	2.50	0.41
1:B:325:GLN:HG3	1:B:332:LYS:HD2	2.02	0.41
1:A:630:THR:CG2	1:A:965:ALA:CB	2.97	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: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:B:558:MET:C	1:B:560:GLN:N	2.74	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:B:269:MET:O	1:B:269:MET:HG2	2.21	0.41
1:A:371:GLU:HA	1:A:371:GLU:OE1	2.21	0.41
1:B:893:ILE:O	1:B:898:LYS:HE3	2.20	0.41
1:B:295:TYR:CD1	1:B:350:CYS:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ARG:HA	1:A:305:PRO:HD3	1.98	0.41
1:B:926:CYS:C	1:B:928:PRO:HD3	2.40	0.41
1:B:496:MET:C	1:B:497:ARG:HG3	2.41	0.41
1:A:570:PRO:HD2	1:A:677:PHE:CZ	2.56	0.41
1:A:922:ILE:HD12	1:A:922:ILE:C	2.41	0.41
1:A:586:ILE:HA	1:A:604:GLY:HA2	2.03	0.41
1:A:474:ASN:HB2	1:A:479:ARG:NH2	2.36	0.41
1:B:953:LYS:HD3	1:B:953:LYS:HA	1.94	0.40
1:B:1043:SER:C	1:B:1045:PRO:HD3	2.41	0.40
1:A:893:ILE:O	1:A:898:LYS:HE3	2.20	0.40
1:A:731:GLU:HG2	1:A:735:LYS:HE3	2.02	0.40
1:B:459:ARG:NE	1:B:492:GLU:OE1	2.54	0.40
1:A:552:ARG:O	1:A:553:MET:C	2.60	0.40
1:B:456:LYS:H	1:B:456:LYS:HG2	1.62	0.40
1:A:927:VAL:O	1:A:928:PRO:C	2.59	0.40
1:B:221:LEU:HD12	1:B:554:LEU:HB2	2.03	0.40
1:B:371:GLU:OE1	1:B:371:GLU:HA	2.21	0.40
1:A:479:ARG:NH1	1:A:479:ARG:HG2	2.35	0.40
1:A:217:ARG:HH21	1:A:551:GLU:HG2	1.85	0.40
1:A:821:LEU:HD11	1:A:934:LEU:HD21	2.02	0.40
1:B:961:ARG:HD2	1:B:961:ARG:H	1.86	0.40
1:A:457:HIS:CD2	1:A:472:LYS:NZ	2.90	0.40
1:B:604:GLY:CA	1:B:955:LEU:HD12	2.37	0.40
1:A:901:LEU:O	1:A:905:HIS:ND1	2.51	0.40
1:B:419:ILE:CG2	1:B:422:MET:HB2	2.52	0.40
1:A:212:ILE:CG2	1:A:260:LEU:HG	2.51	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%)	26	72
1	B	816/852 (96%)	775 (95%)	34 (4%)	7 (1%)	21	68
All	All	1632/1704 (96%)	1549 (95%)	70 (4%)	13 (1%)	24	70

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
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%)	723 (96%)	31 (4%)	37	75
1	B	754/777 (97%)	729 (97%)	25 (3%)	45	80
All	All	1508/1554 (97%)	1452 (96%)	56 (4%)	41	77

All (56) 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	428	ASN
1	A	458	GLU
1	A	463	LEU
1	A	479	ARG
1	A	500	GLN
1	A	510	TYR
1	A	544	LEU
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	930	PHE
1	A	955	LEU
1	A	966	GLU
1	A	973	GLN
1	A	999	ASN
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	428	ASN
1	B	458	GLU
1	B	463	LEU
1	B	479	ARG
1	B	510	TYR
1	B	544	LEU

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Mol	Chain	Res	Type
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	930	PHE
1	B	945	PRO
1	B	966	GLU
1	B	999	ASN
1	B	1045	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	ASN
1	A	276	HIS
1	A	359	GLN
1	A	375	GLN
1	A	428	ASN
1	A	457	HIS
1	A	477	GLN
1	A	500	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	860	GLN
1	A	879	ASN
1	A	905	HIS
1	A	999	ASN
1	B	240	ASN
1	B	244	ASN
1	B	276	HIS
1	B	359	GLN
1	B	428	ASN

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Mol	Chain	Res	Type
1	B	457	HIS
1	B	477	GLN
1	B	585	ASN
1	B	695	HIS
1	B	712	GLN
1	B	860	GLN
1	B	905	HIS
1	B	951	HIS
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 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	824/852 (96%)	0.14	43 (5%)	31 20	35, 135, 288, 306	0
1	B	824/852 (96%)	0.21	55 (6%)	21 12	29, 143, 289, 306	0
All	All	1648/1704 (96%)	0.18	98 (5%)	26 15	29, 139, 289, 306	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	750	HIS	14.6
1	A	751	ASN	9.9
1	A	1045	PRO	9.0
1	B	751	ASN	8.8
1	A	752	ILE	8.0
1	B	1046	ARG	7.8
1	A	481	PRO	6.4
1	A	658	ALA	6.4
1	B	948	LEU	5.4
1	A	1044	ASN	5.4
1	A	662	ALA	4.9
1	A	1035	LEU	4.8
1	B	484	SER	4.6
1	A	657	GLU	4.4
1	B	658	ALA	4.3
1	B	949	LYS	4.3
1	A	667	ASP	4.3
1	A	928	PRO	4.3
1	A	666	GLY	4.3
1	A	656	THR	4.2
1	A	1034	PRO	4.1
1	A	754	PHE	4.1
1	B	950	ARG	4.0
1	B	656	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	950	ARG	4.0
1	B	520	ASP	3.8
1	A	659	ASP	3.7
1	A	479	ARG	3.7
1	B	753	THR	3.6
1	B	486	ALA	3.5
1	A	480	LEU	3.5
1	A	809	TRP	3.5
1	B	1045	PRO	3.5
1	B	569	LEU	3.4
1	B	588	PHE	3.3
1	B	655	PRO	3.3
1	A	948	LEU	3.3
1	B	489	ARG	3.3
1	B	722	ARG	3.3
1	B	750	HIS	3.3
1	B	570	PRO	3.3
1	B	514	PHE	3.3
1	A	753	THR	3.2
1	A	876	SER	3.2
1	A	665	ASN	3.2
1	A	653	PRO	3.1
1	B	526	PHE	3.1
1	A	523	SER	3.1
1	A	500	GLN	3.0
1	B	659	ASP	3.0
1	B	599	PRO	3.0
1	B	653	PRO	3.0
1	B	805	VAL	2.9
1	A	668	GLN	2.9
1	B	479	ARG	2.8
1	B	587	ILE	2.8
1	B	619	ALA	2.8
1	B	810	THR	2.8
1	B	564	GLU	2.7
1	A	755	GLN	2.7
1	B	657	GLU	2.7
1	A	957	ASN	2.7
1	B	668	GLN	2.6
1	A	619	ALA	2.6
1	B	667	ASP	2.6
1	B	568	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	955	LEU	2.5
1	A	655	PRO	2.5
1	B	662	ALA	2.5
1	B	752	ILE	2.5
1	B	590	GLU	2.5
1	B	483	ALA	2.4
1	B	482	GLY	2.4
1	A	320	ALA	2.4
1	A	681	TYR	2.4
1	A	204	LEU	2.4
1	A	661	ILE	2.4
1	A	654	GLU	2.3
1	B	430	ASP	2.3
1	B	584	GLU	2.3
1	B	782	ILE	2.3
1	B	809	TRP	2.3
1	B	652	GLU	2.3
1	B	670	LEU	2.2
1	A	199	GLN	2.2
1	B	492	GLU	2.2
1	B	650	ILE	2.2
1	B	618	TYR	2.2
1	A	522	ASN	2.2
1	B	470	CYS	2.2
1	A	810	THR	2.1
1	B	429	ILE	2.1
1	A	497	ARG	2.1
1	B	981	LEU	2.1
1	A	515	GLU	2.1
1	B	583	GLU	2.0
1	B	490	LEU	2.0
1	B	669	PRO	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.