



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2024 – 09:14 AM EST

PDB ID : 3KSY
Title : Crystal structure of the Histone domain, DH-PH unit, and catalytic unit of the Ras activator Son of Sevenless (SOS)
Authors : Gureasko, J.; Kuchment, O.; Kuriyan, J.
Deposited on : 2009-11-24
Resolution : 3.18 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

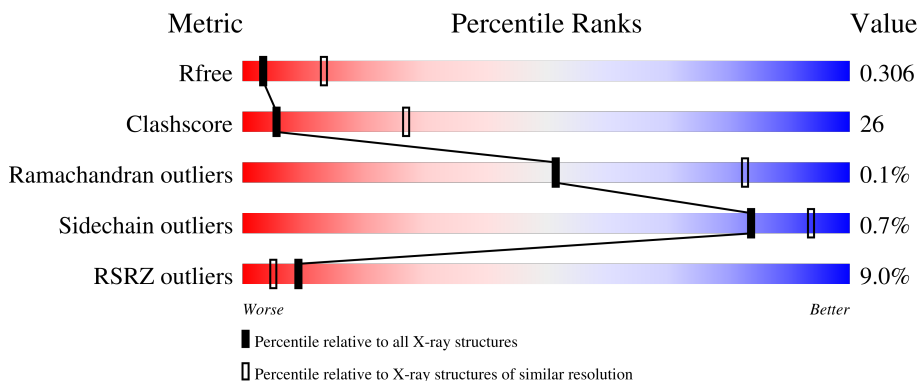
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 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}	130704	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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	1049	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8234 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.

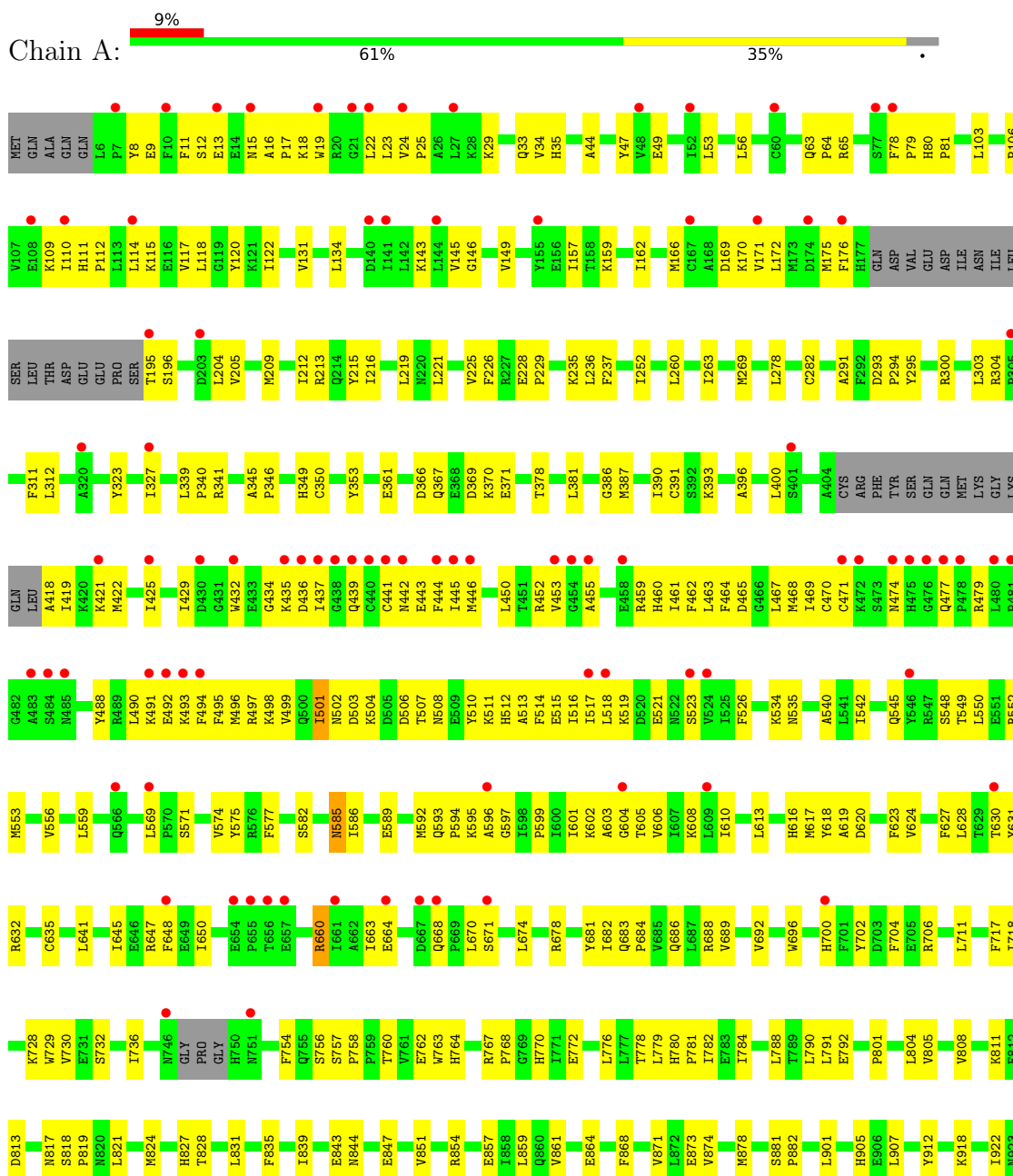
- Molecule 1 is a protein called Son of sevenless homolog 1.

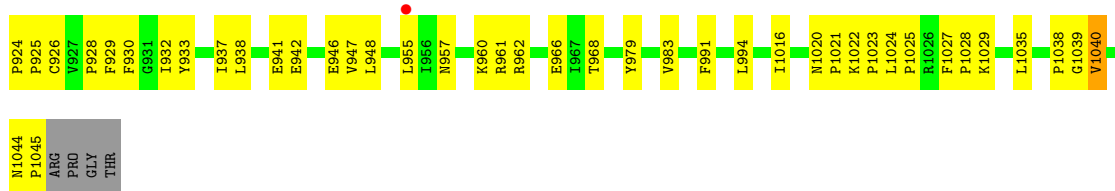
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1007	8234	5259	1411	1527	37	15	0	0

3 Residue-property plots [i](#)

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

- Molecule 1: Son of sevenless homolog 1





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	150.96Å 160.92Å 118.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.81 – 3.18 47.81 – 3.18	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.81-3.18) 99.3 (47.81-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 3.19Å)	Xtrriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.259 , 0.312 0.253 , 0.306	Depositor DCC
R_{free} test set	2000 reflections (8.14%)	wwPDB-VP
Wilson B-factor (Å ²)	92.8	Xtrriage
Anisotropy	0.483	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 93.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8234	wwPDB-VP
Average B, all atoms (Å ²)	139.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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	0.22	0/8413	0.37	0/11363

There are no bond length outliers.

There are no bond angle outliers.

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	8234	0	8242	422	0
All	All	8234	0	8242	422	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (422) 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:445:ILE:HB	1:A:463:LEU:CD2	1.40	1.51
1:A:429:ILE:HG23	1:A:490:LEU:CG	1.64	1.27
1:A:429:ILE:HD12	1:A:490:LEU:HD23	1.22	1.16
1:A:445:ILE:CB	1:A:463:LEU:CD2	2.24	1.15
1:A:518:LEU:HB2	1:A:521:GLU:HB2	1.31	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ILE:HB	1:A:463:LEU:HD22	1.24	1.10
1:A:490:LEU:HD12	1:A:490:LEU:O	1.51	1.10
1:A:445:ILE:HG21	1:A:540:ALA:HB1	1.18	1.09
1:A:445:ILE:CB	1:A:463:LEU:HD22	1.80	1.08
1:A:589:GLU:HB2	1:A:592:MET:SD	1.94	1.06
1:A:445:ILE:HB	1:A:463:LEU:HD21	1.23	1.06
1:A:499:VAL:HG11	1:A:516:ILE:HG23	1.40	1.04
1:A:429:ILE:CG2	1:A:490:LEU:CG	2.36	1.02
1:A:429:ILE:CG2	1:A:490:LEU:HG	1.89	1.02
1:A:514:PHE:CZ	1:A:526:PHE:HB2	1.94	1.01
1:A:514:PHE:HE2	1:A:516:ILE:HD11	1.23	1.00
1:A:429:ILE:CD1	1:A:490:LEU:HD23	1.92	0.98
1:A:429:ILE:HG21	1:A:490:LEU:HD21	1.47	0.96
1:A:429:ILE:HD12	1:A:490:LEU:CD2	1.94	0.96
1:A:445:ILE:CA	1:A:463:LEU:HD22	1.95	0.95
1:A:429:ILE:HG23	1:A:490:LEU:HG	0.96	0.95
1:A:501:ILE:HD13	1:A:501:ILE:H	1.32	0.94
1:A:494:PHE:CE1	1:A:518:LEU:CD2	2.52	0.93
1:A:445:ILE:CB	1:A:463:LEU:HD21	1.94	0.93
1:A:1038:PRO:HB2	1:A:1039:GLY:HA2	1.49	0.92
1:A:495:PHE:HE1	1:A:497:ARG:O	1.53	0.92
1:A:582:SER:H	1:A:585:ASN:HD21	1.17	0.92
1:A:445:ILE:HG21	1:A:540:ALA:CB	1.99	0.92
1:A:494:PHE:CE1	1:A:518:LEU:HD21	2.05	0.92
1:A:501:ILE:HG22	1:A:515:GLU:O	1.69	0.91
1:A:495:PHE:HD1	1:A:497:ARG:H	1.13	0.91
1:A:518:LEU:CB	1:A:521:GLU:HB2	1.99	0.91
1:A:464:PHE:CE2	1:A:469:ILE:HD12	2.06	0.90
1:A:494:PHE:CD1	1:A:518:LEU:HD22	2.07	0.88
1:A:432:TRP:CZ2	1:A:493:LYS:HD3	2.09	0.88
1:A:425:ILE:CD1	1:A:464:PHE:HZ	1.87	0.88
1:A:429:ILE:CG2	1:A:490:LEU:HD21	2.03	0.87
1:A:494:PHE:CD1	1:A:518:LEU:CD2	2.58	0.86
1:A:429:ILE:CG2	1:A:490:LEU:CD2	2.54	0.86
1:A:464:PHE:HE2	1:A:469:ILE:HD12	1.40	0.86
1:A:495:PHE:CE1	1:A:497:ARG:O	2.30	0.85
1:A:461:ILE:HG23	1:A:469:ILE:O	1.75	0.85
1:A:499:VAL:CG1	1:A:516:ILE:HG23	2.07	0.84
1:A:503:ASP:CB	1:A:513:ALA:O	2.25	0.84
1:A:518:LEU:HD13	1:A:521:GLU:OE1	1.77	0.84
1:A:425:ILE:CD1	1:A:464:PHE:CZ	2.61	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ILE:N	1:A:463:LEU:HD22	1.92	0.83
1:A:514:PHE:CE2	1:A:516:ILE:HD11	2.12	0.83
1:A:445:ILE:HG22	1:A:446:MET:HG3	1.58	0.82
1:A:445:ILE:CG2	1:A:540:ALA:HB1	2.07	0.82
1:A:460:HIS:HB3	1:A:471:CYS:SG	2.18	0.82
1:A:514:PHE:CE1	1:A:526:PHE:HB2	2.15	0.81
1:A:269:MET:HG3	1:A:729:TRP:HE1	1.45	0.81
1:A:501:ILE:HD11	1:A:542:ILE:HD11	1.63	0.81
1:A:828:THR:HG23	1:A:873:GLU:HG2	1.61	0.81
1:A:490:LEU:O	1:A:490:LEU:CD1	2.30	0.80
1:A:425:ILE:HD12	1:A:464:PHE:CZ	2.18	0.79
1:A:516:ILE:HD12	1:A:526:PHE:CE2	2.18	0.78
1:A:432:TRP:CE3	1:A:490:LEU:HD21	2.18	0.78
1:A:434:GLY:HA3	1:A:493:LYS:HE3	1.64	0.78
1:A:446:MET:CE	1:A:540:ALA:HB3	2.13	0.78
1:A:503:ASP:HB3	1:A:513:ALA:O	1.83	0.78
1:A:446:MET:HE2	1:A:463:LEU:CD1	2.14	0.78
1:A:514:PHE:HE2	1:A:516:ILE:CD1	1.96	0.77
1:A:491:LYS:HG2	1:A:492:GLU:HG3	1.66	0.77
1:A:514:PHE:CZ	1:A:526:PHE:CB	2.67	0.77
1:A:518:LEU:HB2	1:A:521:GLU:CB	2.14	0.77
1:A:450:LEU:HD12	1:A:461:ILE:HD12	1.65	0.77
1:A:463:LEU:HD23	1:A:463:LEU:C	2.04	0.77
1:A:452:ARG:O	1:A:455:ALA:HB3	1.84	0.76
1:A:419:ILE:HG21	1:A:422:MET:HG3	1.65	0.76
1:A:441:CYS:SG	1:A:467:LEU:HB2	2.26	0.76
1:A:628:LEU:HB3	1:A:700:HIS:CE1	2.21	0.76
1:A:498:LYS:O	1:A:498:LYS:HG2	1.87	0.75
1:A:494:PHE:CE1	1:A:518:LEU:HD22	2.21	0.74
1:A:445:ILE:CG1	1:A:463:LEU:HD21	2.18	0.74
1:A:429:ILE:CG2	1:A:490:LEU:CD1	2.66	0.74
1:A:463:LEU:HD23	1:A:464:PHE:N	2.03	0.74
1:A:429:ILE:HG23	1:A:490:LEU:CD2	2.17	0.73
1:A:444:PHE:HA	1:A:464:PHE:HA	1.68	0.73
1:A:429:ILE:CG2	1:A:490:LEU:HD11	2.18	0.73
1:A:63:GLN:HA	1:A:118:LEU:HD11	1.69	0.73
1:A:446:MET:H	1:A:463:LEU:HB3	1.53	0.73
1:A:429:ILE:HG21	1:A:490:LEU:CD2	2.18	0.72
1:A:754:PHE:CE1	1:A:758:PRO:HG3	2.24	0.72
1:A:445:ILE:HB	1:A:463:LEU:CG	2.19	0.72
1:A:445:ILE:H	1:A:463:LEU:HD22	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ILE:O	1:A:166:MET:HG2	1.89	0.72
1:A:514:PHE:CE2	1:A:526:PHE:HD2	2.07	0.72
1:A:683:GLN:HB3	1:A:684:PRO:HD3	1.70	0.72
1:A:425:ILE:HD13	1:A:464:PHE:CZ	2.23	0.72
1:A:782:ILE:HG22	1:A:861:VAL:HG21	1.71	0.71
1:A:571:SER:HB3	1:A:574:VAL:HG22	1.71	0.71
1:A:491:LYS:NZ	1:A:492:GLU:OE2	2.23	0.71
1:A:516:ILE:HD12	1:A:526:PHE:HE2	1.56	0.71
1:A:754:PHE:HE1	1:A:758:PRO:HG3	1.54	0.71
1:A:432:TRP:CE3	1:A:490:LEU:CD2	2.75	0.70
1:A:432:TRP:CZ3	1:A:490:LEU:HD22	2.26	0.70
1:A:444:PHE:HB3	1:A:464:PHE:CD1	2.27	0.69
1:A:429:ILE:HG21	1:A:432:TRP:HE3	1.57	0.69
1:A:501:ILE:HD13	1:A:501:ILE:N	2.06	0.69
1:A:429:ILE:HG21	1:A:490:LEU:HD11	1.74	0.69
1:A:432:TRP:HE3	1:A:490:LEU:HD21	1.57	0.69
1:A:764:HIS:HB2	1:A:778:THR:O	1.92	0.69
1:A:517:ILE:HG12	1:A:523:SER:OG	1.93	0.69
1:A:446:MET:HE1	1:A:540:ALA:HB3	1.74	0.68
1:A:516:ILE:O	1:A:523:SER:CB	2.42	0.68
1:A:432:TRP:HZ3	1:A:490:LEU:HD22	1.59	0.68
1:A:444:PHE:HB3	1:A:464:PHE:CE1	2.29	0.68
1:A:170:LYS:HD2	1:A:498:LYS:H	1.59	0.67
1:A:425:ILE:HD13	1:A:464:PHE:HZ	1.58	0.67
1:A:501:ILE:HD11	1:A:542:ILE:CD1	2.23	0.67
1:A:501:ILE:HA	1:A:515:GLU:O	1.94	0.67
1:A:425:ILE:HG21	1:A:464:PHE:CZ	2.28	0.67
1:A:445:ILE:HB	1:A:463:LEU:CD1	2.23	0.67
1:A:471:CYS:HB2	1:A:488:TYR:HB3	1.76	0.67
1:A:516:ILE:O	1:A:523:SER:HA	1.95	0.66
1:A:56:LEU:HD13	1:A:134:LEU:HD11	1.77	0.66
1:A:34:VAL:HG11	1:A:143:LYS:HA	1.78	0.66
1:A:149:VAL:HG21	1:A:157:ILE:HG12	1.77	0.66
1:A:79:PRO:HG2	1:A:171:VAL:HG13	1.78	0.65
1:A:418:ALA:HB1	1:A:419:ILE:HG12	1.79	0.65
1:A:446:MET:O	1:A:463:LEU:HB3	1.96	0.65
1:A:446:MET:HE2	1:A:540:ALA:HB3	1.80	0.64
1:A:601:ILE:HD11	1:A:623:PHE:CE1	2.31	0.64
1:A:215:TYR:CE2	1:A:219:LEU:HD11	2.33	0.64
1:A:516:ILE:O	1:A:523:SER:HB3	1.98	0.64
1:A:19:TRP:HB3	1:A:53:LEU:HD21	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ILE:CG2	1:A:540:ALA:CB	2.72	0.63
1:A:494:PHE:HD1	1:A:518:LEU:HD22	1.62	0.62
1:A:593:GLN:HB3	1:A:596:ALA:O	1.98	0.62
1:A:857:GLU:HB3	1:A:1040:VAL:HG21	1.80	0.62
1:A:779:LEU:HB2	1:A:784:ILE:HD11	1.80	0.62
1:A:468:MET:CB	1:A:496:MET:SD	2.88	0.62
1:A:516:ILE:O	1:A:523:SER:CA	2.48	0.62
1:A:445:ILE:H	1:A:463:LEU:CD2	2.12	0.62
1:A:436:ASP:O	1:A:439:GLN:HG2	2.00	0.61
1:A:782:ILE:HG23	1:A:1040:VAL:HA	1.81	0.61
1:A:1038:PRO:CB	1:A:1039:GLY:HA2	2.24	0.61
1:A:462:PHE:HD2	1:A:469:ILE:HG21	1.64	0.61
1:A:429:ILE:HG13	1:A:490:LEU:HD21	1.83	0.61
1:A:1020:ASN:HB3	1:A:1021:PRO:HD3	1.83	0.61
1:A:446:MET:CE	1:A:540:ALA:CB	2.79	0.61
1:A:859:LEU:HD21	1:A:871:VAL:HG13	1.82	0.61
1:A:868:PHE:HZ	1:A:922:ILE:HG13	1.65	0.60
1:A:24:VAL:HB	1:A:25:PRO:HD3	1.83	0.60
1:A:595:LYS:N	1:A:596:ALA:HA	2.15	0.60
1:A:704:PHE:HB3	1:A:711:LEU:HB2	1.83	0.60
1:A:444:PHE:HB2	1:A:463:LEU:O	2.02	0.59
1:A:467:LEU:HD23	1:A:468:MET:N	2.17	0.59
1:A:429:ILE:CD1	1:A:490:LEU:CD2	2.66	0.59
1:A:452:ARG:O	1:A:455:ALA:CB	2.50	0.59
1:A:861:VAL:HA	1:A:864:GLU:HG2	1.84	0.59
1:A:341:ARG:HH22	1:A:535:ASN:HB3	1.67	0.59
1:A:463:LEU:CD2	1:A:463:LEU:C	2.71	0.59
1:A:575:TYR:OH	1:A:647:ARG:HD2	2.03	0.58
1:A:847:GLU:HA	1:A:1035:LEU:HD21	1.85	0.58
1:A:425:ILE:HG21	1:A:464:PHE:HZ	1.67	0.58
1:A:619:ALA:HB2	1:A:688:ARG:HE	1.68	0.58
1:A:221:LEU:HD11	1:A:550:LEU:HB3	1.86	0.58
1:A:11:PHE:N	1:A:12:SER:HA	2.18	0.58
1:A:429:ILE:CG1	1:A:490:LEU:HD21	2.34	0.58
1:A:514:PHE:CE2	1:A:526:PHE:CD2	2.91	0.58
1:A:103:LEU:HD13	1:A:131:VAL:HB	1.84	0.57
1:A:616:HIS:CE1	1:A:617:MET:HG2	2.39	0.57
1:A:762:GLU:HG3	1:A:782:ILE:HD11	1.86	0.57
1:A:110:ILE:O	1:A:114:LEU:HG	2.05	0.57
1:A:1040:VAL:HG12	1:A:1040:VAL:O	2.04	0.57
1:A:516:ILE:HD12	1:A:526:PHE:CD2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:LEU:HD12	1:A:461:ILE:CD1	2.33	0.57
1:A:464:PHE:CE2	1:A:469:ILE:CD1	2.85	0.57
1:A:501:ILE:H	1:A:501:ILE:CD1	2.14	0.57
1:A:696:TRP:HA	1:A:700:HIS:CD2	2.40	0.57
1:A:432:TRP:CZ3	1:A:490:LEU:CD2	2.88	0.57
1:A:501:ILE:CG2	1:A:515:GLU:O	2.50	0.56
1:A:349:HIS:CD2	1:A:353:TYR:HE1	2.23	0.56
1:A:511:LYS:O	1:A:512:HIS:C	2.44	0.56
1:A:278:LEU:HD22	1:A:369:ASP:HB2	1.87	0.56
1:A:474:ASN:HB2	1:A:479:ARG:HH21	1.70	0.56
1:A:702:TYR:O	1:A:706:ARG:HG3	2.05	0.56
1:A:204:LEU:HD12	1:A:205:VAL:N	2.20	0.56
1:A:660:ARG:O	1:A:663:ILE:HG22	2.06	0.56
1:A:991:PHE:HA	1:A:994:LEU:HG	1.85	0.56
1:A:212:ILE:O	1:A:216:ILE:HG13	2.04	0.56
1:A:429:ILE:CG1	1:A:490:LEU:CD2	2.84	0.56
1:A:595:LYS:HB2	1:A:596:ALA:C	2.26	0.56
1:A:630:THR:OG1	1:A:961:ARG:HB3	2.05	0.56
1:A:495:PHE:HD1	1:A:497:ARG:N	1.94	0.56
1:A:663:ILE:HG23	1:A:664:GLU:HG3	1.89	0.55
1:A:65:ARG:HG2	1:A:120:TYR:CE1	2.40	0.55
1:A:441:CYS:SG	1:A:467:LEU:CB	2.95	0.55
1:A:434:GLY:HA3	1:A:493:LYS:CE	2.33	0.55
1:A:435:LYS:HB3	1:A:439:GLN:HG3	1.87	0.55
1:A:781:PRO:HG3	1:A:854:ARG:HD2	1.88	0.55
1:A:684:PRO:HB3	1:A:688:ARG:HH12	1.70	0.55
1:A:80:HIS:CG	1:A:81:PRO:HA	2.41	0.55
1:A:429:ILE:HG21	1:A:432:TRP:CE3	2.40	0.55
1:A:918:LYS:O	1:A:922:ILE:HG12	2.06	0.55
1:A:209:MET:O	1:A:213:ARG:HG3	2.07	0.55
1:A:432:TRP:HE3	1:A:490:LEU:CD2	2.15	0.55
1:A:782:ILE:HG22	1:A:861:VAL:CG2	2.36	0.54
1:A:519:LYS:O	1:A:521:GLU:HG3	2.07	0.54
1:A:495:PHE:O	1:A:496:MET:HB2	2.07	0.54
1:A:514:PHE:CZ	1:A:526:PHE:CD2	2.95	0.54
1:A:9:GLU:HB2	1:A:12:SER:OG	2.08	0.54
1:A:446:MET:N	1:A:463:LEU:HB3	2.23	0.54
1:A:63:GLN:N	1:A:64:PRO:HD3	2.23	0.53
1:A:445:ILE:O	1:A:446:MET:HG3	2.07	0.53
1:A:929:PHE:HD2	1:A:932:ILE:HG12	1.72	0.53
1:A:503:ASP:HB2	1:A:513:ALA:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:LEU:HD13	1:A:678:ARG:NH2	2.23	0.53
1:A:106:PRO:O	1:A:110:ILE:HG13	2.09	0.53
1:A:252:ILE:HG23	1:A:295:TYR:CZ	2.44	0.53
1:A:514:PHE:CE1	1:A:526:PHE:CB	2.88	0.52
1:A:780:HIS:ND1	1:A:782:ILE:HG12	2.24	0.52
1:A:459:ARG:HA	1:A:471:CYS:O	2.09	0.52
1:A:494:PHE:CD1	1:A:518:LEU:HD21	2.33	0.52
1:A:868:PHE:CZ	1:A:922:ILE:HG13	2.44	0.52
1:A:221:LEU:O	1:A:225:VAL:HB	2.09	0.52
1:A:925:PRO:HG3	1:A:979:TYR:HA	1.90	0.52
1:A:425:ILE:HD12	1:A:464:PHE:CE1	2.44	0.51
1:A:668:GLN:HG2	1:A:670:LEU:H	1.74	0.51
1:A:776:LEU:HD23	1:A:851:VAL:HG13	1.92	0.51
1:A:575:TYR:CE2	1:A:577:PHE:HB2	2.45	0.51
1:A:907:LEU:O	1:A:912:TYR:HA	2.09	0.51
1:A:627:PHE:O	1:A:631:TYR:HB3	2.10	0.51
1:A:585:ASN:HD22	1:A:585:ASN:H	1.57	0.51
1:A:170:LYS:HG3	1:A:545:GLN:CD	2.31	0.51
1:A:386:GLY:O	1:A:390:ILE:HG13	2.10	0.51
1:A:788:LEU:O	1:A:792:GLU:HG3	2.11	0.51
1:A:226:PHE:O	1:A:229:PRO:HD2	2.11	0.51
1:A:498:LYS:O	1:A:498:LYS:CG	2.58	0.51
1:A:111:HIS:HB3	1:A:112:PRO:HD3	1.93	0.51
1:A:474:ASN:CB	1:A:479:ARG:HH21	2.24	0.51
1:A:518:LEU:CD1	1:A:521:GLU:OE1	2.56	0.51
1:A:604:GLY:HA2	1:A:955:LEU:HD12	1.92	0.51
1:A:300:ARG:O	1:A:304:ARG:HG3	2.11	0.51
1:A:831:LEU:HD23	1:A:873:GLU:OE1	2.10	0.51
1:A:446:MET:HE2	1:A:540:ALA:CB	2.39	0.50
1:A:504:LYS:HB2	1:A:506:ASP:OD1	2.11	0.50
1:A:818:SER:HB3	1:A:821:LEU:HB3	1.93	0.50
1:A:926:CYS:HA	1:A:979:TYR:OH	2.10	0.50
1:A:808:VAL:HB	1:A:817:ASN:HD22	1.77	0.50
1:A:228:GLU:HB3	1:A:229:PRO:HD3	1.92	0.50
1:A:696:TRP:HD1	1:A:700:HIS:HB2	1.77	0.50
1:A:847:GLU:OE2	1:A:1029:LYS:HB3	2.11	0.50
1:A:1044:ASN:HB2	1:A:1045:PRO:HD3	1.92	0.50
1:A:467:LEU:CD2	1:A:469:ILE:HG13	2.42	0.50
1:A:790:LEU:HD13	1:A:983:VAL:HG22	1.94	0.50
1:A:445:ILE:O	1:A:446:MET:CG	2.60	0.50
1:A:501:ILE:N	1:A:501:ILE:CD1	2.71	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1038:PRO:HB2	1:A:1039:GLY:CA	2.32	0.50
1:A:8:TYR:CG	1:A:117:VAL:HG22	2.46	0.50
1:A:648:PHE:HB2	1:A:689:VAL:HG11	1.93	0.50
1:A:946:GLU:HG3	1:A:947:VAL:HG13	1.93	0.50
1:A:269:MET:HG3	1:A:729:TRP:NE1	2.22	0.49
1:A:788:LEU:HD21	1:A:991:PHE:CD1	2.47	0.49
1:A:23:LEU:HD11	1:A:53:LEU:HD13	1.94	0.49
1:A:599:PRO:HG2	1:A:618:TYR:CZ	2.48	0.49
1:A:632:ARG:HA	1:A:635:CYS:O	2.12	0.49
1:A:912:TYR:CG	1:A:932:ILE:HD11	2.47	0.49
1:A:361:GLU:HG2	1:A:370:LYS:HG3	1.95	0.49
1:A:857:GLU:HB3	1:A:1040:VAL:CG2	2.42	0.49
1:A:429:ILE:HG21	1:A:490:LEU:CD1	2.37	0.49
1:A:446:MET:HE2	1:A:463:LEU:HD12	1.94	0.49
1:A:645:ILE:HG12	1:A:717:PHE:CE1	2.48	0.49
1:A:619:ALA:CB	1:A:688:ARG:HE	2.24	0.49
1:A:425:ILE:HG21	1:A:464:PHE:CE2	2.48	0.49
1:A:462:PHE:HB3	1:A:464:PHE:CE2	2.48	0.49
1:A:804:LEU:HD21	1:A:930:PHE:CZ	2.48	0.49
1:A:432:TRP:CZ2	1:A:493:LYS:CD	2.91	0.48
1:A:933:TYR:O	1:A:937:ILE:HG13	2.12	0.48
1:A:791:LEU:HD22	1:A:827:HIS:CE1	2.48	0.48
1:A:696:TRP:CD1	1:A:704:PHE:CE1	3.01	0.48
1:A:465:ASP:OD1	1:A:465:ASP:O	2.30	0.48
1:A:589:GLU:HG2	1:A:602:LYS:HB2	1.95	0.48
1:A:780:HIS:CE1	1:A:782:ILE:HG12	2.48	0.48
1:A:595:LYS:HB2	1:A:597:GLY:N	2.28	0.48
1:A:29:LYS:O	1:A:33:GLN:HG2	2.14	0.48
1:A:170:LYS:HG3	1:A:545:GLN:HG3	1.96	0.48
1:A:170:LYS:HZ3	1:A:497:ARG:HG2	1.79	0.48
1:A:260:LEU:O	1:A:263:ILE:HG22	2.14	0.48
1:A:295:TYR:HB3	1:A:387:MET:HE1	1.96	0.48
1:A:421:LYS:CB	1:A:444:PHE:CE2	2.96	0.48
1:A:47:TYR:CD1	1:A:159:LYS:HE3	2.48	0.47
1:A:507:THR:HG23	1:A:508:ASN:OD1	2.14	0.47
1:A:169:ASP:O	1:A:170:LYS:HD3	2.14	0.47
1:A:236:LEU:HD22	1:A:237:PHE:CE2	2.49	0.47
1:A:445:ILE:CG1	1:A:463:LEU:CD2	2.83	0.47
1:A:16:ALA:H	1:A:17:PRO:HD2	1.79	0.47
1:A:419:ILE:HG21	1:A:422:MET:CG	2.38	0.47
1:A:620:ASP:O	1:A:624:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LYS:HG2	1:A:122:ILE:HG12	1.97	0.47
1:A:445:ILE:C	1:A:446:MET:HG3	2.35	0.47
1:A:811:LYS:HG2	1:A:813:ASP:H	1.80	0.47
1:A:419:ILE:CD1	1:A:422:MET:SD	3.04	0.46
1:A:432:TRP:HE3	1:A:490:LEU:HD11	1.80	0.46
1:A:170:LYS:HG3	1:A:545:GLN:CG	2.45	0.46
1:A:378:THR:HA	1:A:381:LEU:HG	1.97	0.46
1:A:495:PHE:CD1	1:A:497:ARG:N	2.71	0.46
1:A:512:HIS:HB3	1:A:534:LYS:HB2	1.95	0.46
1:A:585:ASN:HD22	1:A:586:ILE:N	2.13	0.46
1:A:941:GLU:HA	1:A:960:LYS:HE3	1.97	0.46
1:A:601:ILE:HD11	1:A:623:PHE:HE1	1.79	0.46
1:A:605:THR:CG2	1:A:608:LYS:HD3	2.45	0.46
1:A:115:LYS:HE2	1:A:122:ILE:H	1.80	0.46
1:A:460:HIS:O	1:A:471:CYS:SG	2.73	0.46
1:A:549:THR:O	1:A:553:MET:HG3	2.15	0.46
1:A:593:GLN:HB2	1:A:596:ALA:HB1	1.98	0.46
1:A:660:ARG:C	1:A:660:ARG:HE	2.19	0.46
1:A:295:TYR:C	1:A:387:MET:HE1	2.35	0.46
1:A:924:PRO:HA	1:A:925:PRO:C	2.36	0.46
1:A:106:PRO:HB2	1:A:109:LYS:HB2	1.96	0.45
1:A:175:MET:HG3	1:A:176:PHE:CD1	2.51	0.45
1:A:452:ARG:HB3	1:A:455:ALA:CB	2.46	0.45
1:A:764:HIS:HB3	1:A:780:HIS:N	2.31	0.45
1:A:548:SER:O	1:A:552:ARG:HG3	2.17	0.45
1:A:628:LEU:O	1:A:700:HIS:HE1	1.98	0.45
1:A:15:ASN:HB3	1:A:18:LYS:HD2	1.99	0.45
1:A:801:PRO:HB3	1:A:968:THR:HB	1.97	0.45
1:A:393:LYS:HB3	1:A:396:ALA:HB3	1.99	0.45
1:A:589:GLU:HB2	1:A:592:MET:CG	2.45	0.45
1:A:446:MET:HB2	1:A:463:LEU:HD13	1.99	0.45
1:A:818:SER:N	1:A:819:PRO:HD3	2.31	0.45
1:A:844:ASN:HB2	1:A:1028:PRO:O	2.17	0.45
1:A:303:LEU:HD13	1:A:396:ALA:HB1	1.99	0.45
1:A:901:LEU:HG	1:A:905:HIS:CE1	2.52	0.45
1:A:195:THR:HA	1:A:196:SER:HA	1.50	0.45
1:A:477:GLN:O	1:A:479:ARG:HD2	2.17	0.45
1:A:835:PHE:O	1:A:839:ILE:HG13	2.17	0.44
1:A:682:ILE:HG23	1:A:686:GLN:CD	2.37	0.44
1:A:422:MET:HE1	1:A:441:CYS:O	2.16	0.44
1:A:429:ILE:HD12	1:A:490:LEU:CG	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ILE:HD12	1:A:463:LEU:HD21	1.99	0.44
1:A:445:ILE:CD1	1:A:463:LEU:HD21	2.48	0.44
1:A:295:TYR:CD2	1:A:350:CYS:HB2	2.51	0.44
1:A:462:PHE:HD2	1:A:469:ILE:CG2	2.30	0.44
1:A:467:LEU:C	1:A:496:MET:HG3	2.37	0.44
1:A:696:TRP:CD1	1:A:704:PHE:HE1	2.35	0.44
1:A:962:ARG:O	1:A:966:GLU:HG2	2.18	0.44
1:A:35:HIS:CE1	1:A:146:GLY:HA3	2.53	0.44
1:A:569:LEU:HD12	1:A:569:LEU:H	1.82	0.44
1:A:453:VAL:HG11	1:A:510:TYR:HE2	1.82	0.44
1:A:681:TYR:O	1:A:684:PRO:HD2	2.17	0.44
1:A:16:ALA:N	1:A:17:PRO:HD2	2.33	0.44
1:A:470:CYS:O	1:A:490:LEU:CB	2.65	0.44
1:A:843:GLU:HA	1:A:1016:ILE:HG22	1.99	0.44
1:A:44:ALA:HB1	1:A:162:ILE:HD11	2.00	0.43
1:A:421:LYS:CB	1:A:444:PHE:HE2	2.31	0.43
1:A:613:LEU:HG	1:A:692:VAL:HG11	2.01	0.43
1:A:682:ILE:HG23	1:A:686:GLN:NE2	2.34	0.43
1:A:762:GLU:HG3	1:A:782:ILE:CD1	2.47	0.43
1:A:784:ILE:HG23	1:A:991:PHE:CZ	2.53	0.43
1:A:391:CYS:HB3	1:A:400:LEU:HD11	2.00	0.43
1:A:585:ASN:HD22	1:A:585:ASN:N	2.13	0.43
1:A:732:SER:O	1:A:736:ILE:HD13	2.18	0.43
1:A:418:ALA:HA	1:A:419:ILE:HA	1.41	0.43
1:A:323:TYR:O	1:A:327:ILE:HG12	2.18	0.43
1:A:429:ILE:HG13	1:A:490:LEU:CD2	2.47	0.43
1:A:462:PHE:HB2	1:A:469:ILE:HB	2.00	0.43
1:A:756:SER:HA	1:A:757:SER:HA	1.75	0.43
1:A:419:ILE:HD13	1:A:422:MET:SD	2.58	0.43
1:A:518:LEU:HB3	1:A:521:GLU:OE1	2.18	0.43
1:A:718:ILE:CG2	1:A:730:VAL:HG13	2.49	0.43
1:A:603:ALA:HB2	1:A:957:ASN:HA	2.01	0.42
1:A:881:SER:HB2	1:A:882:PRO:HD3	1.99	0.42
1:A:345:ALA:HB3	1:A:346:PRO:HD3	2.01	0.42
1:A:291:ALA:O	1:A:294:PRO:HD2	2.20	0.42
1:A:630:THR:HG22	1:A:805:VAL:HG21	2.00	0.42
1:A:938:LEU:HD23	1:A:941:GLU:OE2	2.19	0.42
1:A:991:PHE:HD1	1:A:994:LEU:HD11	1.84	0.42
1:A:172:LEU:N	1:A:172:LEU:HD12	2.35	0.42
1:A:293:ASP:N	1:A:294:PRO:CD	2.82	0.42
1:A:79:PRO:CG	1:A:171:VAL:HG13	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:PHE:HB2	1:A:469:ILE:HD12	2.00	0.42
1:A:339:LEU:HB3	1:A:340:PRO:HD3	2.02	0.42
1:A:444:PHE:CB	1:A:463:LEU:O	2.68	0.42
1:A:575:TYR:CE1	1:A:650:ILE:HG12	2.54	0.42
1:A:641:LEU:O	1:A:645:ILE:HG13	2.20	0.42
1:A:684:PRO:CB	1:A:688:ARG:HH12	2.32	0.42
1:A:767:ARG:HB2	1:A:770:HIS:CE1	2.55	0.42
1:A:569:LEU:HD12	1:A:569:LEU:N	2.35	0.42
1:A:624:VAL:HG13	1:A:692:VAL:HG12	2.01	0.42
1:A:881:SER:N	1:A:882:PRO:CD	2.83	0.42
1:A:518:LEU:HB3	1:A:521:GLU:HB2	1.95	0.41
1:A:559:LEU:HD23	1:A:559:LEU:O	2.20	0.41
1:A:831:LEU:HG	1:A:835:PHE:CE2	2.55	0.41
1:A:955:LEU:HD22	1:A:955:LEU:N	2.35	0.41
1:A:474:ASN:HB2	1:A:479:ARG:NH2	2.35	0.41
1:A:514:PHE:CE2	1:A:526:PHE:HB2	2.51	0.41
1:A:593:GLN:HA	1:A:594:PRO:HD3	1.76	0.41
1:A:425:ILE:O	1:A:429:ILE:HG12	2.20	0.41
1:A:602:LYS:HE3	1:A:948:LEU:HD11	2.02	0.41
1:A:9:GLU:OE1	1:A:13:GLU:HB2	2.20	0.41
1:A:366:ASP:HB3	1:A:369:ASP:HB3	2.03	0.41
1:A:432:TRP:HE3	1:A:490:LEU:CD1	2.33	0.41
1:A:763:TRP:CZ3	1:A:768:PRO:HB3	2.56	0.41
1:A:1022:LYS:HA	1:A:1023:PRO:HD3	1.90	0.41
1:A:22:LEU:H	1:A:22:LEU:HD23	1.85	0.41
1:A:847:GLU:O	1:A:851:VAL:HG23	2.20	0.41
1:A:1024:LEU:HD23	1:A:1025:PRO:O	2.19	0.41
1:A:78:PHE:HA	1:A:79:PRO:HD3	1.93	0.41
1:A:311:PHE:HD2	1:A:312:LEU:HD12	1.86	0.41
1:A:432:TRP:CH2	1:A:493:LYS:HD3	2.51	0.41
1:A:938:LEU:HB3	1:A:942:GLU:OE2	2.21	0.41
1:A:145:VAL:O	1:A:149:VAL:HG23	2.20	0.41
1:A:282:CYS:HA	1:A:728:LYS:NZ	2.36	0.41
1:A:435:LYS:O	1:A:436:ASP:C	2.59	0.41
1:A:442:ASN:O	1:A:443:GLU:CG	2.69	0.41
1:A:502:ASN:H	1:A:515:GLU:HB3	1.86	0.41
1:A:437:ILE:HG23	1:A:467:LEU:HD13	2.02	0.41
1:A:442:ASN:C	1:A:443:GLU:HG3	2.41	0.41
1:A:671:SER:HB3	1:A:674:LEU:HD12	2.03	0.41
1:A:843:GLU:HB3	1:A:1027:PHE:CG	2.55	0.40
1:A:874:VAL:O	1:A:878:MET:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:GLN:O	1:A:371:GLU:HG2	2.21	0.40
1:A:552:ARG:O	1:A:556:VAL:HG23	2.21	0.40
1:A:606:VAL:O	1:A:610:ILE:HG13	2.22	0.40
1:A:11:PHE:HB3	1:A:12:SER:CA	2.52	0.40
1:A:23:LEU:HD12	1:A:49:GLU:HB2	2.03	0.40
1:A:824:MET:HB3	1:A:824:MET:HE2	1.94	0.40
1:A:926:CYS:O	1:A:928:PRO:HD3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	999/1049 (95%)	957 (96%)	41 (4%)	1 (0%)	51 83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1040	VAL

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	914/955 (96%)	908 (99%)	6 (1%)	84 93

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	235	LYS
1	A	501	ILE
1	A	585	ASN
1	A	660	ARG
1	A	760	THR
1	A	772	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	HIS
1	A	244	ASN
1	A	375	GLN
1	A	477	GLN
1	A	585	ASN
1	A	700	HIS
1	A	817	ASN
1	A	827	HIS
1	A	830	ASN
1	A	860	GLN
1	A	973	GLN

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 monosaccharides 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	1007/1049 (95%)	0.51	91 (9%) 9 5	44, 128, 261, 402	4 (0%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	481	PRO	10.6
1	A	493	LYS	9.0
1	A	21	GLY	7.2
1	A	484	SER	7.1
1	A	439	GLN	6.9
1	A	10	PHE	6.9
1	A	478	PRO	6.5
1	A	425	ILE	5.9
1	A	440	CYS	5.9
1	A	475	HIS	5.7
1	A	436	ASP	5.5
1	A	566	GLN	5.5
1	A	480	LEU	5.1
1	A	455	ALA	5.1
1	A	114	LEU	5.1
1	A	485	ASN	5.0
1	A	667	ASP	4.9
1	A	435	LYS	4.8
1	A	477	GLN	4.7
1	A	494	PHE	4.7
1	A	78	PHE	4.6
1	A	654	GLU	4.4
1	A	492	GLU	4.3
1	A	746	ASN	4.2
1	A	445	ILE	4.1
1	A	27	LEU	3.9
1	A	421	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	471	CYS	3.8
1	A	441	CYS	3.8
1	A	454	GLY	3.7
1	A	320	ALA	3.7
1	A	518	LEU	3.7
1	A	664	GLU	3.7
1	A	437	ILE	3.7
1	A	596	ALA	3.6
1	A	442	ASN	3.5
1	A	155	TYR	3.5
1	A	671	SER	3.5
1	A	22	LEU	3.4
1	A	13	GLU	3.4
1	A	438	GLY	3.3
1	A	476	GLY	3.3
1	A	546	TYR	3.3
1	A	195	THR	3.3
1	A	432	TRP	3.1
1	A	569	LEU	3.1
1	A	474	ASN	3.1
1	A	19	TRP	3.1
1	A	458	GLU	3.1
1	A	327	ILE	3.1
1	A	48	VAL	3.1
1	A	108	GLU	3.0
1	A	656	THR	3.0
1	A	52	ILE	3.0
1	A	668	GLN	2.9
1	A	483	ALA	2.8
1	A	655	PRO	2.7
1	A	661	ILE	2.7
1	A	446	MET	2.6
1	A	453	VAL	2.6
1	A	171	VAL	2.6
1	A	657	GLU	2.6
1	A	401	SER	2.6
1	A	524	VAL	2.6
1	A	700	HIS	2.6
1	A	472	LYS	2.5
1	A	140	ASP	2.5
1	A	24	VAL	2.4
1	A	144	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	430	ASP	2.4
1	A	630	THR	2.4
1	A	77	SER	2.4
1	A	305	PRO	2.4
1	A	203	ASP	2.4
1	A	523	SER	2.4
1	A	15	ASN	2.3
1	A	609	LEU	2.3
1	A	60	CYS	2.3
1	A	648	PHE	2.3
1	A	517	ILE	2.3
1	A	491	LYS	2.3
1	A	955	LEU	2.3
1	A	174	ASP	2.2
1	A	110	ILE	2.2
1	A	167	CYS	2.2
1	A	751	ASN	2.1
1	A	176	PHE	2.1
1	A	141	ILE	2.1
1	A	604	GLY	2.1
1	A	7	PRO	2.0
1	A	444	PHE	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 monosaccharides 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.