



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:54 am BST

PDB ID : 4REB
Title : Structural Insights into 5' Flap DNA Unwinding and Incision by the Human FAN1 Dimer
Authors : Zhao, Q.; Xue, X.; Longerich, S.; Sung, P.; Xiong, Y.
Deposited on : 2014-09-22
Resolution : 4.20 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 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	:	2.11
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)	:	2.11

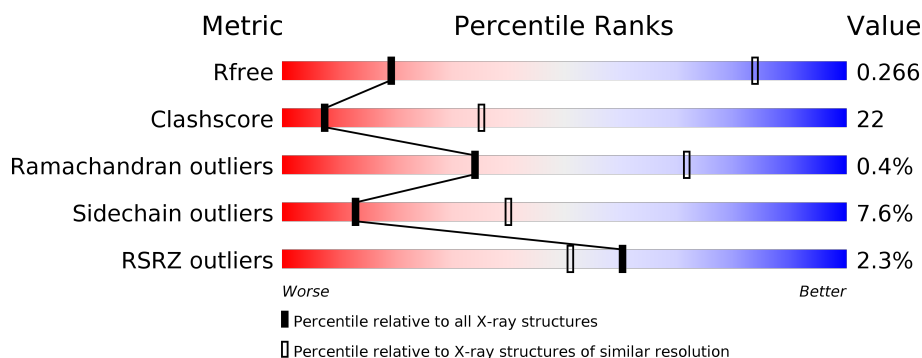
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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	1005 (4.62-3.78)
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)
RSRZ outliers	127900	1063 (4.70-3.70)

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 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	D	9	<div> <div>33%</div> <div>67%</div> </div>
2	E	20	<div> <div>45%</div> <div>55%</div> </div>
3	F	10	<div> <div>50%</div> <div>50%</div> </div>
4	A	647	<div> <div>2%</div> <div>56%</div> <div>27%</div> <div>13%</div> </div>
4	H	647	<div> <div>2%</div> <div>55%</div> <div>32%</div> <div>10%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10114 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 DNA chain called DNA (5'-D(P*GP*TP*GP*GP*CP*GP*AP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	9	Total	C	N	O	P	0	0	0
			189	88	38	54	9			

- Molecule 2 is a DNA chain called DNA (5'-D(P*CP*GP*TP*GP*GP*CP*GP*AP*GP*CP*GP*CP*TP*CP*GP*CP*CP*AP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	20	Total	C	N	O	P	0	0	0
			410	192	78	120	20			

- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*CP*TP*CP*GP*CP*CP*AP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	10	Total	C	N	O	P	0	0	0
			202	95	37	60	10			

- Molecule 4 is a protein called Fanconi-associated nuclease 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	566	Total	C	N	O	S	0	1	0
			4590	2931	815	821	23			
4	H	584	Total	C	N	O	S	0	1	0
			4721	3014	841	843	23			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	371	GLU	-	EXPRESSION TAG	UNP Q9Y2M0
A	372	PHE	-	EXPRESSION TAG	UNP Q9Y2M0
A	960	ALA	ASP	ENGINEERED MUTATION	UNP Q9Y2M0
H	371	GLU	-	EXPRESSION TAG	UNP Q9Y2M0

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Chain	Residue	Modelled	Actual	Comment	Reference
H	372	PHE	-	EXPRESSION TAG	UNP Q9Y2M0
H	960	ALA	ASP	ENGINEERED MUTATION	UNP Q9Y2M0

- Molecule 5 is SAMARIUM (III) ION (three-letter code: SM) (formula: Sm).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total 1	Sm 1	0	0
5	A	1	Total 1	Sm 1	0	0

3 Residue-property plots [i](#)

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

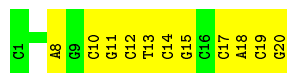
- Molecule 1: DNA (5'-D(P*GP*TP*GP*GP*CP*GP*AP*GP*C)-3')

Chain D: 



- Molecule 2: DNA (5'-D(P*CP*GP*TP*GP*GP*CP*GP*AP*GP*CP*GP*CP*TP*CP*GP*C P*CP*AP*CP*G)-3')

Chain E: 



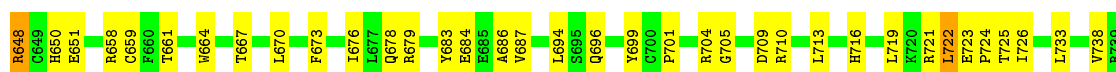
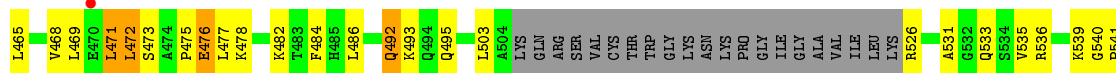
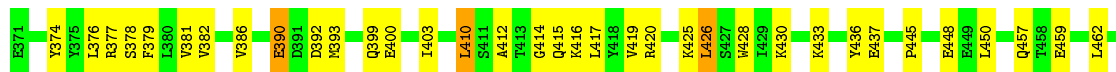
- Molecule 3: DNA (5'-D(P*GP*CP*TP*CP*GP*CP*CP*AP*CP*G)-3')

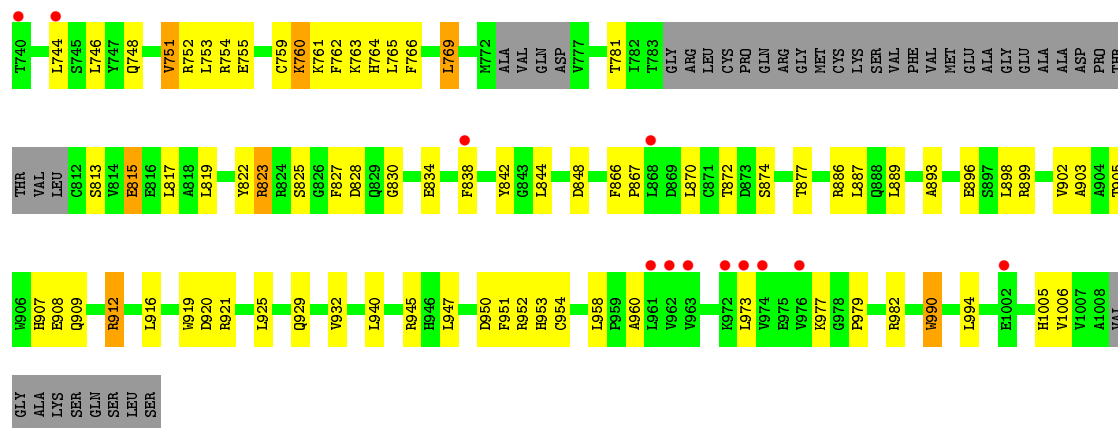
Chain F: 



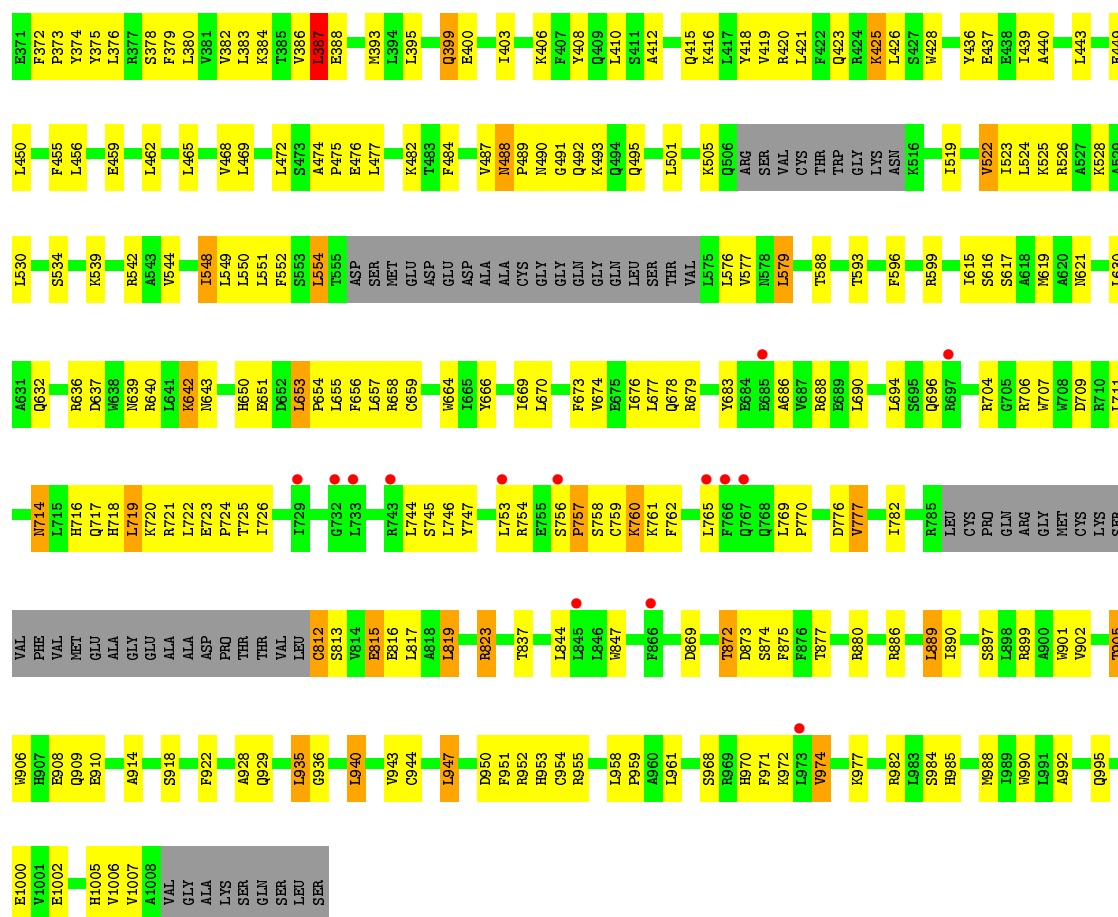
- Molecule 4: Fanconi-associated nuclease 1

Chain A: 





• Molecule 4: Fanconi-associated nuclease 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	104.77Å 104.77Å 127.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	90.70 – 4.20 90.73 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (90.70-4.20) 99.3 (90.73-4.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 4.15Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.230 , 0.262 0.240 , 0.266	Depositor DCC
R_{free} test set	566 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	247.1	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 248.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.196 for -h,-k,l 0.359 for h,-h-k,-l 0.198 for -k,-h,-l	Xtriage
Reported twinning fraction	0.495 for H, K, L 0.505 for K, H, -L	Depositor
Outliers	0 of 11360 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10114	wwPDB-VP
Average B, all atoms (Å ²)	297.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SM

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	D	0.49	0/212	0.84	1/326 (0.3%)
2	E	0.44	0/459	0.75	0/706
3	F	0.48	0/225	0.75	0/344
4	A	0.57	0/4689	0.79	6/6339 (0.1%)
4	H	0.57	0/4822	0.80	3/6518 (0.0%)
All	All	0.56	0/10407	0.79	10/14233 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	421	LEU	CB-CG-CD2	-6.66	99.68	111.00
4	A	471	LEU	CA-CB-CG	6.04	129.18	115.30
4	H	889	LEU	CA-CB-CG	5.80	128.63	115.30
4	A	630	LEU	CB-CG-CD2	5.79	120.85	111.00
4	H	387	LEU	CA-CB-CG	5.79	128.61	115.30
4	A	472	LEU	CA-CB-CG	5.78	128.59	115.30
4	A	633	CYS	CA-CB-SG	5.59	124.06	114.00
1	D	5	DG	C1'-O4'-C4'	-5.45	104.65	110.10
4	A	547	ARG	NE-CZ-NH2	-5.39	117.61	120.30
4	A	472	LEU	CB-CG-CD1	5.27	119.96	111.00

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	D	189	0	101	6	0
2	E	410	0	223	13	1
3	F	202	0	112	3	0
4	A	4590	0	4602	205	1
4	H	4721	0	4752	214	2
5	A	1	0	0	0	0
5	H	1	0	0	0	0
All	All	10114	0	9790	431	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 (431) 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)
4:A:579:LEU:HB2	4:A:582:MET:CE	1.39	1.47
4:A:579:LEU:HA	4:A:582:MET:CG	1.43	1.47
4:H:374:TYR:CE2	4:H:577:VAL:HG13	1.52	1.42
4:A:579:LEU:CA	4:A:582:MET:HG2	1.50	1.36
4:A:579:LEU:CB	4:A:582:MET:CE	2.12	1.26
4:H:717:GLN:O	4:H:720:LYS:HG2	1.17	1.23
4:A:755:GLU:OE2	4:H:482:LYS:HE3	1.39	1.22
4:A:579:LEU:CB	4:A:582:MET:HE1	1.80	1.09
4:H:374:TYR:CE2	4:H:577:VAL:CG1	2.38	1.05
4:A:579:LEU:HB3	4:A:582:MET:HE1	1.44	0.98
4:H:717:GLN:O	4:H:720:LYS:CG	2.11	0.97
4:A:644:HIS:CE1	4:A:646:SER:H	1.84	0.95
4:H:577:VAL:O	4:H:579:LEU:HD12	1.67	0.93
4:A:579:LEU:HB2	4:A:582:MET:HE2	0.93	0.92
4:A:579:LEU:CB	4:A:582:MET:HE2	1.89	0.90
4:H:376:LEU:HD13	4:H:419:VAL:HG21	1.54	0.90
4:A:912:ARG:HB3	4:A:912:ARG:HH11	1.37	0.89
4:A:459:GLU:HA	4:A:462:LEU:HD13	1.54	0.88
4:A:716:HIS:HB2	4:A:725:THR:HG21	1.53	0.87
4:H:908:GLU:HG3	4:H:909:GLN:HG2	1.57	0.86
4:A:576:LEU:O	4:A:579:LEU:HD23	1.77	0.84
4:H:374:TYR:HE2	4:H:577:VAL:HG13	1.06	0.84
4:A:950:ASP:OD2	4:A:953:HIS:ND1	2.09	0.83
4:A:636:ARG:HH11	4:A:636:ARG:CG	1.92	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:579:LEU:HA	4:A:582:MET:SD	2.20	0.81
4:A:636:ARG:HH11	4:A:636:ARG:HG3	1.45	0.81
4:A:492:GLN:HB3	4:A:495:GLN:HG2	1.62	0.81
4:A:579:LEU:C	4:A:582:MET:HG2	2.01	0.80
4:A:641:LEU:O	4:A:643:ASN:N	2.14	0.80
4:H:823:ARG:HH11	4:H:823:ARG:HG3	1.47	0.79
4:H:653:LEU:HD12	4:H:654:PRO:HD2	1.63	0.79
4:H:677:LEU:HD13	4:H:686:ALA:HB2	1.63	0.78
4:A:755:GLU:HG2	4:A:755:GLU:O	1.83	0.76
4:H:651:GLU:O	4:H:658:ARG:NH2	2.19	0.76
4:A:912:ARG:CB	4:A:912:ARG:HH11	1.98	0.76
4:H:650:HIS:O	4:H:658:ARG:NH1	2.18	0.76
4:A:645:PRO:O	4:A:648:ARG:HB2	1.86	0.75
4:H:418:TYR:CE1	4:H:455:PHE:HB3	2.23	0.74
4:H:935:LEU:HD11	4:H:940:LEU:HD13	1.68	0.74
4:H:576:LEU:O	4:H:579:LEU:HG	1.89	0.73
4:A:579:LEU:HA	4:A:582:MET:HG2	0.75	0.73
4:A:638:TRP:HE1	4:A:642:LYS:HZ2	1.35	0.71
4:A:428:TRP:CH2	4:A:457:GLN:HG3	2.26	0.71
4:A:644:HIS:ND1	4:A:646:SER:N	2.38	0.71
1:D:10:DC:N3	2:E:11:DG:O6	2.25	0.70
4:H:653:LEU:O	4:H:658:ARG:NH1	2.24	0.70
4:H:653:LEU:N	4:H:658:ARG:HH12	1.90	0.70
4:A:909:GLN:HA	4:A:912:ARG:NH2	2.06	0.70
4:A:579:LEU:CA	4:A:582:MET:CG	2.33	0.70
4:A:684:GLU:N	4:A:684:GLU:OE1	2.25	0.70
4:A:755:GLU:OE2	4:H:482:LYS:CE	2.31	0.69
4:H:418:TYR:HE1	4:H:455:PHE:HB3	1.57	0.69
4:H:656:PHE:HB3	4:H:872:THR:HG21	1.75	0.69
4:H:379:PHE:O	4:H:383:LEU:HG	1.92	0.69
4:A:912:ARG:O	4:A:919:TRP:NE1	2.24	0.69
4:H:465:LEU:O	4:H:469:LEU:HG	1.94	0.68
4:A:866:PHE:HB2	4:A:870:LEU:HD22	1.74	0.68
4:H:395:LEU:HD11	4:H:596:PHE:HB2	1.75	0.68
4:H:420:ARG:HG3	4:H:439:ILE:HD11	1.76	0.67
4:A:982:ARG:NH1	4:H:525:LYS:O	2.24	0.67
4:H:716:HIS:NE2	4:H:753:LEU:HG	2.09	0.67
4:A:374:TYR:OH	4:A:577:VAL:CG1	2.43	0.67
4:A:426:LEU:HD11	4:A:542:ARG:CZ	2.25	0.66
4:A:477:LEU:HB3	4:A:493:LYS:HZ2	1.59	0.66
4:H:872:THR:HG23	4:H:874:SER:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:12:DC:H2''	2:E:13:DT:H5'	1.78	0.66
4:A:639[B]:ASN:O	4:A:643:ASN:OD1	2.13	0.66
4:H:677:LEU:HD12	4:H:678:GLN:N	2.11	0.66
4:H:378:SER:HB3	4:H:579:LEU:HD13	1.79	0.65
4:H:484:PHE:HZ	4:H:526:ARG:CZ	2.09	0.65
4:A:410:LEU:HD22	4:A:414:GLY:HA3	1.78	0.65
4:H:637:ASP:HA	4:H:640:ARG:HG2	1.77	0.65
4:H:653:LEU:HD11	4:H:657:LEU:HB2	1.77	0.65
4:A:898:LEU:HD13	4:A:940:LEU:HD12	1.79	0.65
4:A:912:ARG:HB3	4:A:912:ARG:NH1	2.10	0.65
4:H:694:LEU:HD11	4:H:707:TRP:HB3	1.79	0.65
4:H:716:HIS:CD2	4:H:753:LEU:HD11	2.32	0.65
1:D:6:DC:H2''	1:D:7:DG:C8	2.31	0.65
4:H:450:LEU:HB2	4:H:456:LEU:HD23	1.79	0.65
4:H:897:SER:HB3	4:H:901:TRP:CH2	2.32	0.65
4:A:909:GLN:HA	4:A:912:ARG:CZ	2.26	0.64
3:F:26:DC:H2''	3:F:27:DG:C8	2.33	0.64
4:A:705:GLY:HA2	4:A:738:VAL:HG22	1.80	0.64
4:A:659:CYS:HA	4:A:664:TRP:CD2	2.33	0.64
4:A:579:LEU:CB	4:A:582:MET:SD	2.86	0.64
4:H:673:PHE:O	4:H:677:LEU:HG	1.98	0.64
2:E:12:DC:H2'	2:E:13:DT:C6	2.32	0.63
4:A:579:LEU:CA	4:A:582:MET:SD	2.85	0.63
4:H:382:VAL:HG23	4:H:552:PHE:CG	2.32	0.63
4:A:644:HIS:CE1	4:A:645:PRO:HG2	2.33	0.63
4:A:912:ARG:CG	4:A:912:ARG:HH11	2.11	0.63
4:A:639[A]:ASN:O	4:A:643:ASN:OD1	2.16	0.62
4:A:925:LEU:O	4:A:929:GLN:HG2	2.00	0.62
4:H:677:LEU:CD1	4:H:686:ALA:HB2	2.30	0.62
4:H:812:CYS:HB3	4:H:817:LEU:HD11	1.80	0.62
4:H:462:LEU:HG	4:H:468:VAL:HG12	1.81	0.62
4:H:577:VAL:C	4:H:579:LEU:HD12	2.20	0.62
4:H:944:CYS:HA	4:H:947:LEU:HD11	1.82	0.62
4:H:683:TYR:O	4:H:686:ALA:HB3	2.00	0.61
4:H:554:LEU:HD23	4:H:554:LEU:H	1.65	0.61
4:A:374:TYR:OH	4:A:577:VAL:HG11	1.99	0.61
4:A:374:TYR:CE2	4:A:577:VAL:CG1	2.83	0.61
4:H:579:LEU:HD12	4:H:579:LEU:H	1.64	0.61
4:H:813:SER:HB3	4:H:816:GLU:HG2	1.82	0.61
4:H:653:LEU:O	4:H:658:ARG:CZ	2.48	0.61
4:A:641:LEU:C	4:A:643:ASN:H	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:968:SER:OG	4:H:970:HIS:ND1	2.29	0.60
4:A:632:GLN:HE22	4:A:636:ARG:NE	1.99	0.60
4:A:678:GLN:HE22	4:A:710:ARG:HG3	1.65	0.60
4:H:487:VAL:HG23	4:H:488:ASN:ND2	2.16	0.60
2:E:8:DA:H61	3:F:25:DT:H3	1.49	0.60
4:H:539:LYS:O	4:H:542:ARG:HG2	2.02	0.60
4:A:909:GLN:OE1	4:A:912:ARG:NE	2.34	0.60
4:H:639[A]:ASN:O	4:H:642:LYS:HB2	2.02	0.60
4:A:426:LEU:HD12	4:A:426:LEU:N	2.17	0.59
4:H:632:GLN:O	4:H:636:ARG:NH1	2.35	0.59
4:A:723:GLU:HB3	4:A:724:PRO:HD3	1.83	0.59
4:A:638:TRP:HE1	4:A:642:LYS:NZ	2.00	0.59
4:H:723:GLU:HB2	4:H:724:PRO:HD3	1.85	0.59
1:D:10:DC:C4	2:E:11:DG:O6	2.55	0.59
4:H:659:CYS:HA	4:H:664:TRP:CD2	2.37	0.59
4:A:908:GLU:O	4:A:912:ARG:NH2	2.35	0.59
4:H:762:PHE:HB3	4:H:765:LEU:HD12	1.85	0.59
4:A:641:LEU:O	4:A:644:HIS:N	2.36	0.58
4:H:823:ARG:CG	4:H:823:ARG:HH11	2.15	0.58
4:H:984:SER:O	4:H:988:MET:HG3	2.03	0.58
4:A:475:PRO:O	4:A:478:LYS:HG2	2.03	0.58
4:H:386:VAL:HG12	4:H:393:MET:CE	2.33	0.58
4:A:842:TYR:CE2	4:A:951:PHE:HE1	2.21	0.58
4:A:428:TRP:CD2	4:A:536:ARG:HB2	2.39	0.58
4:A:819:LEU:HD21	4:A:830:GLY:HA3	1.86	0.58
4:H:522:VAL:HG22	4:H:526:ARG:HH22	1.68	0.58
1:D:2:DG:N3	2:E:20:DG:N2	2.53	0.57
4:H:721:ARG:NH1	4:H:723:GLU:OE1	2.37	0.57
4:H:477:LEU:HD22	4:H:493:LYS:HD2	1.87	0.57
4:H:954:CYS:HA	4:H:990:TRP:CZ2	2.39	0.57
4:A:579:LEU:O	4:A:582:MET:HG2	2.04	0.57
4:H:462:LEU:CG	4:H:468:VAL:HG12	2.35	0.57
4:H:425:LYS:HD2	4:H:426:LEU:H	1.70	0.56
4:A:430:LYS:O	4:A:433:LYS:HB2	2.05	0.56
4:A:468:VAL:O	4:A:472:LEU:HD22	2.05	0.56
4:A:638:TRP:O	4:A:642:LYS:N	2.30	0.56
4:A:551:LEU:HD21	4:A:602:LEU:HD21	1.86	0.56
4:H:487:VAL:HG23	4:H:488:ASN:HD21	1.70	0.56
4:H:440:ALA:HB3	4:H:443:LEU:HD23	1.87	0.56
4:A:576:LEU:HD13	4:A:577:VAL:N	2.21	0.56
4:H:489:PRO:C	4:H:491:GLY:H	2.07	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:465:LEU:O	4:A:469:LEU:HG	2.06	0.56
4:H:674:VAL:HG13	4:H:690:LEU:HD11	1.85	0.56
4:A:579:LEU:HB2	4:A:582:MET:SD	2.45	0.56
4:H:886:ARG:O	4:H:890:ILE:HG12	2.05	0.56
4:H:579:LEU:HD12	4:H:579:LEU:N	2.21	0.56
4:H:384:LYS:HA	4:H:387:LEU:HG	1.88	0.55
4:H:522:VAL:HG22	4:H:526:ARG:NH2	2.22	0.55
4:H:653:LEU:H	4:H:658:ARG:HH12	1.54	0.55
4:A:576:LEU:O	4:A:579:LEU:HB3	2.07	0.55
4:H:813:SER:O	4:H:817:LEU:HD12	2.06	0.55
4:H:819:LEU:O	4:H:823:ARG:NH1	2.40	0.55
4:H:383:LEU:HD13	4:H:408:TYR:OH	2.07	0.55
4:H:426:LEU:HD22	4:H:542:ARG:HD3	1.89	0.55
4:H:576:LEU:HD23	4:H:576:LEU:N	2.22	0.55
4:H:523:ILE:HA	4:H:526:ARG:HH21	1.72	0.55
4:H:659:CYS:HA	4:H:664:TRP:CG	2.42	0.55
4:A:696:GLN:O	4:A:704:ARG:NH1	2.41	0.54
4:A:576:LEU:HD13	4:A:578:ASN:H	1.73	0.54
4:A:636:ARG:HG3	4:A:636:ARG:NH1	2.20	0.54
4:A:386:VAL:HG12	4:A:393:MET:CE	2.38	0.54
4:A:766:PHE:O	4:A:769:LEU:HG	2.06	0.54
4:A:842:TYR:CE2	4:A:916:LEU:HD13	2.41	0.54
4:H:484:PHE:CZ	4:H:526:ARG:CZ	2.89	0.54
4:H:745:SER:HB2	4:H:985:HIS:CD2	2.42	0.54
4:A:726:ILE:HD13	4:A:753:LEU:HD13	1.89	0.54
4:A:415:GLN:O	4:A:419:VAL:HG23	2.09	0.53
4:A:644:HIS:ND1	4:A:645:PRO:N	2.56	0.53
4:A:412:ALA:O	4:A:416:LYS:HG3	2.08	0.53
4:A:400:GLU:O	4:A:403:ILE:HB	2.08	0.53
4:H:655:LEU:HA	4:H:658:ARG:HB2	1.90	0.53
4:H:754:ARG:HH12	4:H:769:LEU:HD22	1.72	0.53
4:A:374:TYR:CZ	4:A:577:VAL:CG1	2.91	0.53
4:A:667:THR:HA	4:A:670:LEU:HD12	1.90	0.53
4:A:954:CYS:HA	4:A:990:TRP:CZ2	2.43	0.53
2:E:17:DC:H2"	2:E:18:DA:C8	2.44	0.53
4:H:666:TYR:O	4:H:670:LEU:HG	2.09	0.53
4:H:374:TYR:CD2	4:H:577:VAL:HG13	2.33	0.53
4:A:579:LEU:HB3	4:A:582:MET:CE	2.11	0.53
4:A:903:ALA:HB2	4:A:929:GLN:NE2	2.24	0.52
4:A:430:LYS:HG3	4:A:533:GLN:O	2.09	0.52
4:A:886:ARG:O	4:A:889:LEU:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:670:LEU:O	4:H:673:PHE:HB3	2.09	0.52
4:H:459:GLU:HB3	4:H:534:SER:H	1.74	0.52
4:H:819:LEU:C	4:H:823:ARG:HH12	2.12	0.52
4:A:754:ARG:HH11	4:A:754:ARG:HG3	1.75	0.52
4:H:899:ARG:HG2	4:H:929:GLN:HB3	1.91	0.52
4:A:982:ARG:HH12	4:H:525:LYS:C	2.11	0.52
4:A:468:VAL:HA	4:A:471:LEU:HG	1.91	0.52
4:A:642:LYS:HE2	4:A:699:TYR:CE2	2.45	0.52
4:H:639[B]:ASN:O	4:H:642:LYS:HB2	2.09	0.51
4:H:579:LEU:CD1	4:H:579:LEU:H	2.22	0.51
4:A:903:ALA:HB2	4:A:929:GLN:HE22	1.75	0.51
4:A:473:SER:N	4:A:476:GLU:OE2	2.34	0.51
4:H:686:ALA:O	4:H:690:LEU:HD13	2.10	0.51
4:A:400:GLU:HA	4:A:403:ILE:HD12	1.93	0.51
4:H:844:LEU:HD13	4:H:902:VAL:HG13	1.93	0.51
4:A:379:PHE:O	4:A:382:VAL:HG22	2.11	0.51
4:H:465:LEU:O	4:H:468:VAL:HG22	2.11	0.51
4:H:757:PRO:O	4:H:760:LYS:HG2	2.11	0.51
4:H:747:TYR:CE1	4:H:770:PRO:HD2	2.46	0.51
4:H:696:GLN:O	4:H:704:ARG:NH2	2.41	0.51
4:A:644:HIS:CE1	4:A:646:SER:N	2.66	0.50
4:A:374:TYR:CE2	4:A:577:VAL:HG13	2.46	0.50
4:A:748:GLN:O	4:A:751:VAL:HG13	2.10	0.50
4:H:709:ASP:HA	4:H:746:LEU:HD21	1.93	0.50
4:A:374:TYR:CE2	4:A:577:VAL:HG12	2.46	0.50
4:H:501:LEU:O	4:H:505:LYS:HG3	2.12	0.50
4:A:838:PHE:HB2	4:A:958:LEU:HD13	1.94	0.50
4:H:905:THR:HA	4:H:908:GLU:HG2	1.93	0.50
1:D:9:DG:H1	2:E:12:DC:N4	2.09	0.50
4:A:844:LEU:HA	4:A:905:THR:HG21	1.94	0.50
4:H:406:LYS:O	4:H:410:LEU:HG	2.12	0.50
4:A:716:HIS:HB2	4:A:725:THR:CG2	2.35	0.50
4:H:642:LYS:O	4:H:643:ASN:HB2	2.11	0.50
4:H:847:TRP:CH2	4:H:914:ALA:HB2	2.47	0.50
4:A:762:PHE:HA	4:A:764:HIS:CE1	2.47	0.49
4:H:972:LYS:HE2	4:H:1000:GLU:HG2	1.95	0.49
4:H:386:VAL:CG1	4:H:551:LEU:HD11	2.42	0.49
4:A:632:GLN:HE22	4:A:636:ARG:CZ	2.24	0.49
4:H:782:ILE:HD11	4:H:1006:VAL:HG22	1.93	0.49
4:A:726:ILE:HD12	4:A:766:PHE:CZ	2.47	0.49
4:A:889:LEU:O	4:A:893:ALA:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:653:LEU:HD12	4:H:654:PRO:CD	2.37	0.49
4:A:477:LEU:HB3	4:A:493:LYS:NZ	2.27	0.49
4:A:813:SER:O	4:A:817:LEU:HG	2.13	0.49
4:A:842:TYR:HB2	4:A:947:LEU:HD13	1.95	0.49
4:H:400:GLU:O	4:H:403:ILE:HB	2.13	0.49
4:H:378:SER:CB	4:H:579:LEU:HD13	2.41	0.49
4:A:428:TRP:CZ3	4:A:462:LEU:HD11	2.48	0.49
4:A:659:CYS:HA	4:A:664:TRP:CG	2.48	0.49
4:A:887:LEU:HD11	4:A:945:ARG:HB2	1.95	0.49
4:H:961:LEU:HB3	4:H:974:VAL:HG13	1.94	0.49
4:A:428:TRP:CE3	4:A:536:ARG:HB2	2.48	0.49
4:A:459:GLU:HA	4:A:462:LEU:CD1	2.36	0.49
4:A:636:ARG:CG	4:A:636:ARG:NH1	2.61	0.49
4:A:678:GLN:NE2	4:A:710:ARG:HG3	2.27	0.49
4:A:683:TYR:O	4:A:686:ALA:HB3	2.13	0.49
4:H:544:VAL:O	4:H:548:ILE:HG23	2.12	0.49
4:H:944:CYS:HA	4:H:947:LEU:CD1	2.42	0.49
4:A:899:ARG:HG3	4:A:929:GLN:HB3	1.94	0.49
4:A:576:LEU:CD1	4:A:578:ASN:H	2.25	0.49
4:A:661:THR:HG23	4:A:664:TRP:H	1.78	0.49
4:A:823:ARG:NH2	4:A:827:PHE:O	2.34	0.49
4:A:426:LEU:HD21	4:A:542:ARG:HD3	1.95	0.48
4:A:472:LEU:HD12	4:A:476:GLU:OE1	2.13	0.48
4:A:761:LYS:HG2	4:A:761:LYS:H	1.32	0.48
4:H:462:LEU:O	4:H:528:LYS:HD2	2.12	0.48
4:H:462:LEU:CD2	4:H:468:VAL:HG12	2.44	0.48
4:A:754:ARG:NH1	4:A:754:ARG:HG3	2.29	0.48
4:H:716:HIS:HB2	4:H:725:THR:HG21	1.94	0.48
4:H:922:PHE:CD2	4:H:928:ALA:HB2	2.48	0.48
4:H:403:ILE:HG23	4:H:455:PHE:CE1	2.48	0.48
4:A:716:HIS:CB	4:A:725:THR:HG21	2.36	0.48
4:A:642:LYS:HE2	4:A:699:TYR:HE2	1.79	0.48
4:A:902:VAL:HG21	4:A:932:VAL:HG11	1.94	0.48
4:H:716:HIS:NE2	4:H:753:LEU:CG	2.75	0.48
4:H:386:VAL:HG11	4:H:551:LEU:HD11	1.95	0.48
4:A:410:LEU:HB3	4:A:415:GLN:HG3	1.96	0.47
4:H:386:VAL:HG12	4:H:393:MET:HE2	1.96	0.47
4:H:450:LEU:CB	4:H:456:LEU:HD23	2.44	0.47
4:H:374:TYR:CD2	4:H:577:VAL:CG1	2.94	0.47
4:A:842:TYR:HE2	4:A:916:LEU:HD13	1.79	0.47
4:H:395:LEU:HD23	4:H:599:ARG:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:690:LEU:HD23	4:H:711:LEU:HB2	1.96	0.47
4:A:426:LEU:HD12	4:A:426:LEU:H	1.77	0.47
4:A:753:LEU:O	4:A:759:CYS:HB2	2.14	0.47
4:H:412:ALA:O	4:H:416:LYS:HG3	2.14	0.47
4:H:468:VAL:O	4:H:472:LEU:HG	2.14	0.47
4:A:426:LEU:H	4:A:426:LEU:CD1	2.27	0.47
4:A:643:ASN:OD1	4:A:643:ASN:N	2.48	0.47
4:H:462:LEU:HG	4:H:468:VAL:CG1	2.44	0.47
4:H:593:THR:HG21	4:H:653:LEU:HD13	1.96	0.47
4:H:683:TYR:CD1	4:H:718:HIS:CE1	3.02	0.47
4:A:874:SER:HA	4:A:877:THR:OG1	2.15	0.47
4:H:387:LEU:HD23	4:H:408:TYR:OH	2.14	0.47
4:H:637:ASP:HA	4:H:640:ARG:CG	2.44	0.47
4:H:722:LEU:HD13	4:H:759:CYS:SG	2.55	0.47
4:A:579:LEU:HA	4:A:582:MET:CB	2.34	0.47
4:A:678:GLN:HE22	4:A:710:ARG:CG	2.27	0.47
4:A:762:PHE:HB3	4:A:765:LEU:HD12	1.96	0.47
4:A:823:ARG:HE	4:A:828:ASP:HA	1.80	0.47
4:H:437:GLU:N	4:H:437:GLU:OE1	2.45	0.47
4:H:616:SER:HA	4:H:619:MET:HE2	1.97	0.47
4:H:877:THR:HG22	4:H:880:ARG:HH21	1.80	0.47
4:H:943:VAL:O	4:H:947:LEU:HG	2.14	0.47
4:H:387:LEU:HD12	4:H:388:GLU:HG3	1.96	0.47
4:A:390:GLU:HG2	4:A:390:GLU:H	1.42	0.47
4:A:579:LEU:O	4:A:582:MET:N	2.48	0.47
4:A:722:LEU:O	4:A:726:ILE:HG12	2.15	0.47
4:A:760:LYS:O	4:A:763:LYS:HG2	2.14	0.47
4:A:979:PRO:HD3	4:A:1006:VAL:O	2.15	0.47
4:H:428:TRP:CE2	4:H:462:LEU:HD13	2.50	0.47
4:H:488:ASN:O	4:H:491:GLY:N	2.47	0.47
4:H:897:SER:HB3	4:H:901:TRP:CZ2	2.50	0.47
4:H:722:LEU:HD11	4:H:762:PHE:CE2	2.50	0.46
4:H:869:ASP:O	4:H:875:PHE:HB2	2.15	0.46
4:H:423:GLN:OE1	4:H:423:GLN:N	2.47	0.46
4:A:716:HIS:CD2	4:A:753:LEU:HD21	2.49	0.46
4:H:519:ILE:O	4:H:522:VAL:HG13	2.15	0.46
4:H:992:ALA:HA	4:H:995:GLN:HG2	1.97	0.46
4:H:782:ILE:O	4:H:1007:VAL:HG22	2.16	0.46
4:H:951:PHE:CZ	4:H:955:ARG:HD2	2.50	0.46
4:A:417:LEU:HD23	4:A:450:LEU:HD12	1.98	0.46
4:A:540:GLY:N	4:A:541:PRO:CD	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:661:THR:HG22	4:A:664:TRP:HB2	1.97	0.46
4:A:760:LYS:HD2	4:A:760:LYS:HA	1.58	0.46
4:A:887:LEU:HD21	4:A:945:ARG:HH12	1.81	0.46
4:H:415:GLN:O	4:H:419:VAL:HG23	2.15	0.46
4:H:632:GLN:HE21	4:H:673:PHE:HZ	1.63	0.46
4:A:644:HIS:O	4:A:647:LEU:HG	2.16	0.46
4:A:377:ARG:O	4:A:381:VAL:HG23	2.15	0.46
4:H:674:VAL:CG1	4:H:690:LEU:HD11	2.46	0.46
4:H:716:HIS:CD2	4:H:716:HIS:O	2.69	0.46
4:A:430:LYS:NZ	4:A:531:ALA:O	2.28	0.46
4:H:489:PRO:C	4:H:491:GLY:N	2.69	0.46
4:A:650:HIS:CG	4:A:661:THR:OG1	2.69	0.45
4:H:395:LEU:O	4:H:395:LEU:HD23	2.16	0.45
4:H:428:TRP:NE1	4:H:462:LEU:HD13	2.31	0.45
4:H:906:TRP:O	4:H:910:GLU:HB2	2.16	0.45
4:A:445:PRO:HA	4:A:448:GLU:OE1	2.16	0.45
4:H:722:LEU:O	4:H:726:ILE:HG12	2.15	0.45
4:A:426:LEU:HD11	4:A:542:ARG:NE	2.31	0.45
4:A:912:ARG:CG	4:A:912:ARG:NH1	2.76	0.45
1:D:9:DG:N2	2:E:12:DC:N3	2.62	0.45
4:H:922:PHE:HD2	4:H:928:ALA:HB2	1.81	0.45
4:A:834:GLU:HG3	4:A:960:ALA:HA	1.99	0.45
4:H:690:LEU:O	4:H:694:LEU:HD13	2.17	0.45
4:H:759:CYS:HA	4:H:762:PHE:CD2	2.51	0.45
4:H:420:ARG:HG3	4:H:439:ILE:CD1	2.45	0.45
4:H:759:CYS:HA	4:H:762:PHE:HD2	1.82	0.44
4:H:935:LEU:HA	4:H:971:PHE:CE1	2.52	0.44
4:A:392:ASP:CG	4:A:591:ARG:HH12	2.21	0.44
4:A:842:TYR:CE2	4:A:951:PHE:CE1	3.03	0.44
4:H:382:VAL:O	4:H:386:VAL:HG23	2.17	0.44
4:H:747:TYR:CD1	4:H:770:PRO:HD2	2.53	0.44
2:E:12:DC:H2''	2:E:13:DT:C5'	2.47	0.44
4:H:974:VAL:HA	4:H:1002:GLU:O	2.18	0.44
4:A:896:GLU:OE2	4:A:899:ARG:HD2	2.18	0.44
4:H:420:ARG:HD3	4:H:436:TYR:CD1	2.52	0.44
4:A:403:ILE:HD13	4:A:544:VAL:HG21	1.99	0.44
4:A:579:LEU:C	4:A:582:MET:H	2.20	0.44
4:H:399:GLN:HG2	4:H:400:GLU:N	2.32	0.44
4:H:462:LEU:HB3	4:H:528:LYS:HE3	1.99	0.44
4:A:761:LYS:HG3	4:A:762:PHE:CE2	2.53	0.44
4:A:848:ASP:OD1	4:A:886:ARG:NH2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:10:DC:H2"	2:E:11:DG:OP2	2.18	0.44
4:H:522:VAL:CG2	4:H:526:ARG:HH12	2.30	0.44
4:A:426:LEU:CD1	4:A:426:LEU:N	2.80	0.44
4:H:373:PRO:HB2	4:H:375:TYR:CE2	2.53	0.44
4:H:372:PHE:CD1	4:H:372:PHE:O	2.71	0.44
4:A:973:LEU:HD12	4:A:994:LEU:HD13	2.00	0.43
4:H:523:ILE:HA	4:H:526:ARG:NH2	2.32	0.43
4:H:714:ASN:O	4:H:719:LEU:HB2	2.18	0.43
4:H:813:SER:OG	4:H:815:GLU:HG2	2.18	0.43
4:H:387:LEU:HD12	4:H:388:GLU:N	2.33	0.43
4:H:476:GLU:HB3	4:H:530:LEU:HD13	2.00	0.43
4:H:474:ALA:N	4:H:475:PRO:HD2	2.34	0.43
4:A:719:LEU:HD13	4:A:721:ARG:CZ	2.48	0.43
4:A:822:TYR:HA	4:A:825:SER:HB2	2.00	0.43
4:H:950:ASP:CG	4:H:953:HIS:HD1	2.21	0.43
2:E:14:DC:H2"	2:E:15:DG:C8	2.53	0.43
4:H:677:LEU:HD12	4:H:678:GLN:H	1.83	0.43
4:H:823:ARG:NH1	4:H:823:ARG:CG	2.78	0.43
3:F:31:DC:H2"	3:F:32:DG:C8	2.53	0.43
4:H:548:ILE:HG13	4:H:549:LEU:N	2.34	0.43
4:H:936:GLY:O	4:H:940:LEU:HD22	2.19	0.43
4:A:374:TYR:HE2	4:A:577:VAL:HG13	1.82	0.43
4:A:459:GLU:CA	4:A:462:LEU:HD13	2.38	0.42
4:A:815:GLU:HG2	4:A:815:GLU:H	1.55	0.42
4:A:465:LEU:O	4:A:468:VAL:HG12	2.19	0.42
4:A:644:HIS:CG	4:A:645:PRO:HD2	2.55	0.42
4:A:673:PHE:HA	4:A:676:ILE:HD12	2.01	0.42
4:A:920:ASP:N	4:A:920:ASP:OD1	2.52	0.42
4:A:694:LEU:HA	4:A:704:ARG:NH1	2.35	0.42
4:A:716:HIS:CE1	4:A:753:LEU:HG	2.54	0.42
4:A:781:THR:HG22	4:A:1005:HIS:HB2	2.01	0.42
4:H:577:VAL:O	4:H:579:LEU:CD1	2.53	0.42
4:H:958:LEU:HA	4:H:959:PRO:HD3	1.91	0.42
4:A:651:GLU:O	4:A:658:ARG:NH1	2.50	0.42
4:H:420:ARG:HD3	4:H:436:TYR:CE1	2.54	0.42
4:H:815:GLU:HB3	4:H:961:LEU:HD21	2.01	0.42
4:H:380:LEU:HD22	4:H:383:LEU:HD11	2.02	0.42
4:A:709:ASP:HA	4:A:746:LEU:HD21	2.00	0.42
4:A:716:HIS:O	4:A:716:HIS:CD2	2.73	0.42
4:H:716:HIS:CE1	4:H:753:LEU:HG	2.54	0.42
4:H:615:ILE:HD11	4:H:630:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:382:VAL:HG13	4:H:383:LEU:N	2.35	0.41
4:H:837:THR:HG23	4:H:922:PHE:HE1	1.85	0.41
4:A:416:LYS:O	4:A:420:ARG:HG3	2.20	0.41
4:A:576:LEU:HD13	4:A:577:VAL:H	1.86	0.41
4:H:677:LEU:HD13	4:H:686:ALA:CB	2.42	0.41
4:H:382:VAL:HG23	4:H:552:PHE:CD1	2.55	0.41
4:H:410:LEU:HD22	4:H:449:GLU:HG2	2.00	0.41
4:H:673:PHE:HA	4:H:676:ILE:HD12	2.02	0.41
4:H:379:PHE:O	4:H:382:VAL:HG12	2.21	0.41
4:H:462:LEU:HD21	4:H:468:VAL:HG12	2.02	0.41
4:H:716:HIS:CD2	4:H:753:LEU:HD21	2.56	0.41
4:A:701:PRO:O	4:A:704:ARG:HG2	2.20	0.41
4:H:655:LEU:O	4:H:658:ARG:HB2	2.21	0.41
4:H:658:ARG:HH11	4:H:658:ARG:HG2	1.86	0.41
4:A:492:GLN:CB	4:A:495:GLN:HG2	2.40	0.41
4:A:899:ARG:HG3	4:A:929:GLN:CD	2.40	0.41
4:A:921:ARG:HA	4:A:921:ARG:HD3	1.72	0.41
4:H:666:TYR:CD1	4:H:669:ILE:HD12	2.56	0.41
4:H:756:SER:O	4:H:758:SER:N	2.53	0.41
4:A:410:LEU:O	4:A:415:GLN:NE2	2.54	0.41
4:A:710:ARG:NH1	4:A:713:LEU:HD22	2.35	0.41
4:A:977:LYS:O	4:A:1005:HIS:HA	2.21	0.41
4:H:488:ASN:N	4:H:489:PRO:HD3	2.36	0.41
2:E:12:DC:H2'	2:E:13:DT:H6	1.84	0.41
4:H:395:LEU:CD2	4:H:599:ARG:HA	2.51	0.41
4:A:484:PHE:CD2	4:A:503:LEU:HD21	2.56	0.40
4:A:687:VAL:HG21	4:A:719:LEU:HD11	2.03	0.40
4:H:776:ASP:OD1	4:H:776:ASP:N	2.54	0.40
4:H:977:LYS:O	4:H:1005:HIS:HA	2.21	0.40
4:A:420:ARG:HD3	4:A:436:TYR:CE1	2.57	0.40
4:A:733:LEU:HD23	4:A:733:LEU:HA	1.89	0.40
4:H:492:GLN:O	4:H:495:GLN:HG2	2.21	0.40
4:A:425:LYS:HG3	4:A:426:LEU:N	2.36	0.40
4:A:867:PRO:HG2	4:A:870:LEU:HD13	2.03	0.40
4:H:465:LEU:HD23	4:H:501:LEU:HD23	2.04	0.40
4:A:658:ARG:O	4:A:661:THR:HG22	2.21	0.40
4:A:912:ARG:HG2	4:A:912:ARG:HH11	1.83	0.40
4:H:380:LEU:CD2	4:H:383:LEU:HD11	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)
4:A:580:GLY:O	4:H:688:ARG:NH2[3_664]	1.97	0.23
2:E:19:DC:OP2	4:H:436:TYR:OH[2_545]	2.07	0.13

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
4	A	557/647 (86%)	539 (97%)	17 (3%)	1 (0%)	47 81
4	H	577/647 (89%)	552 (96%)	22 (4%)	3 (0%)	29 68
All	All	1134/1294 (88%)	1091 (96%)	39 (3%)	4 (0%)	34 72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	642	LYS
4	H	490	ASN
4	H	757	PRO
4	H	777	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
4	A	498/562 (89%)	459 (92%)	39 (8%)	12 39
4	H	511/562 (91%)	473 (93%)	38 (7%)	13 40
All	All	1009/1124 (90%)	932 (92%)	77 (8%)	13 40

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	376	LEU
4	A	378	SER
4	A	390	GLU
4	A	399	GLN
4	A	410	LEU
4	A	426	LEU
4	A	437	GLU
4	A	476	GLU
4	A	482	LYS
4	A	486	LEU
4	A	492	GLN
4	A	526	ARG
4	A	535	VAL
4	A	539	LYS
4	A	542	ARG
4	A	576	LEU
4	A	579	LEU
4	A	593	THR
4	A	602	LEU
4	A	632	GLN
4	A	636	ARG
4	A	640	ARG
4	A	642	LYS
4	A	643	ASN
4	A	648	ARG
4	A	679	ARG
4	A	722	LEU
4	A	744	LEU
4	A	751	VAL
4	A	752	ARG
4	A	760	LYS
4	A	769	LEU
4	A	815	GLU
4	A	823	ARG
4	A	872	THR
4	A	907	HIS
4	A	912	ARG
4	A	952	ARG
4	A	990	TRP
4	H	387	LEU
4	H	399	GLN
4	H	425	LYS

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Mol	Chain	Res	Type
4	H	488	ASN
4	H	522	VAL
4	H	524	LEU
4	H	548	ILE
4	H	550	LEU
4	H	554	LEU
4	H	579	LEU
4	H	588	THR
4	H	617	SER
4	H	621	ASN
4	H	642	LYS
4	H	653	LEU
4	H	679	ARG
4	H	706	ARG
4	H	714	ASN
4	H	719	LEU
4	H	744	LEU
4	H	760	LYS
4	H	761	LYS
4	H	777	VAL
4	H	812	CYS
4	H	815	GLU
4	H	819	LEU
4	H	823	ARG
4	H	872	THR
4	H	873	ASP
4	H	889	LEU
4	H	905	THR
4	H	918	SER
4	H	935	LEU
4	H	940	LEU
4	H	947	LEU
4	H	952	ARG
4	H	974	VAL
4	H	982	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	678	GLN
4	A	714	ASN
4	H	678	GLN

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Mol	Chain	Res	Type
4	H	714	ASN
4	H	718	HIS

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	D	9/9 (100%)	-0.70	0 100 100	292, 298, 305, 312	0
2	E	20/20 (100%)	-0.54	0 100 100	268, 286, 307, 312	0
3	F	10/10 (100%)	-0.29	0 100 100	248, 263, 328, 352	0
4	A	566/647 (87%)	-0.18	13 (2%) 60 51	243, 294, 353, 396	0
4	H	584/647 (90%)	-0.17	14 (2%) 59 49	218, 299, 364, 449	0
All	All	1189/1333 (89%)	-0.19	27 (2%) 60 51	218, 295, 358, 449	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	962	VAL	4.6
4	H	753	LEU	3.6
4	A	963	VAL	3.6
4	A	1002	GLU	3.5
4	H	685	GLU	3.5
4	H	845	LEU	3.4
4	A	973	LEU	3.2
4	H	756	SER	3.1
4	H	697	ARG	3.0
4	H	743	ARG	2.9
4	A	740	THR	2.7
4	A	961	LEU	2.7
4	H	766	PHE	2.5
4	A	974	VAL	2.5
4	H	729	ILE	2.4
4	H	733	LEU	2.4
4	H	767	GLN	2.4
4	H	732	GLY	2.4
4	H	765	LEU	2.4
4	H	866	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
4	A	972	LYS	2.2
4	A	838	PHE	2.1
4	A	976	VAL	2.1
4	A	744	LEU	2.1
4	A	470	GLU	2.1
4	A	868	LEU	2.0
4	H	973	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SM	A	1101	1/1	0.91	0.30	340,340,340,340	0
5	SM	H	1101	1/1	0.94	0.26	386,386,386,386	0

6.5 Other polymers [i](#)

There are no such residues in this entry.