



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 03:37 am BST

PDB ID : 4REA
Title : A Nuclease DNA complex
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Deposited on : 2014-09-22
Resolution : 3.81 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

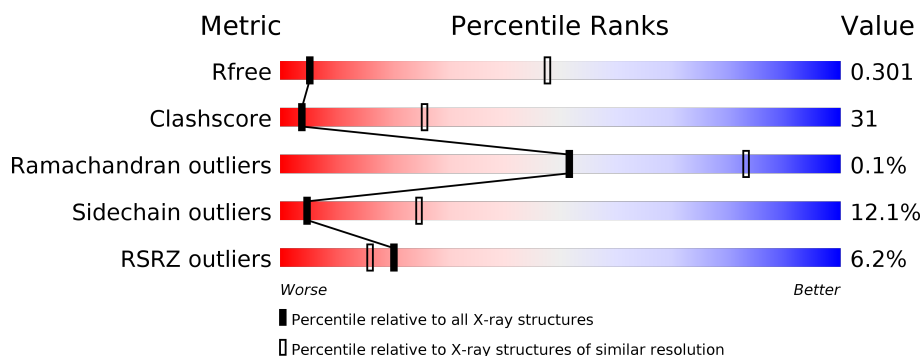
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.81 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	1231 (4.04-3.60)
Clashscore	141614	1031 (4.02-3.62)
Ramachandran outliers	138981	1261 (4.04-3.60)
Sidechain outliers	138945	1255 (4.04-3.60)
RSRZ outliers	127900	1139 (4.04-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	647	<div> <div>7%</div> <div>52%</div> <div>35%</div> <div>•</div> <div>9%</div> </div>
1	B	647	<div> <div>4%</div> <div>51%</div> <div>34%</div> <div>6%</div> <div>9%</div> </div>
2	C	10	<div> <div>20%</div> <div>80%</div> </div>
3	D	10	<div> <div>10%</div> <div>90%</div> </div>
4	E	17	<div> <div>18%</div> <div>24%</div> <div>76%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10270 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 Fanconi-associated nuclease 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	588	Total	C	N	O	S	0	1	0
			4752	3031	841	856	24			
1	A	590	Total	C	N	O	S	0	1	0
			4764	3039	846	854	25			

There are 6 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	P	0	0	0
			197	95	34	59	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	10	Total	C	N	O	P	0	0	0
			208	97	41	60	10			

- Molecule 4 is a DNA chain called DNA (5'-D(P*GP*GP*CP*GP*AP*GP*CP*GP*CP*TP*CP*GP*CP*CP*AP*CP*G)-3').

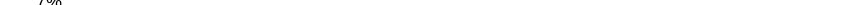
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	17	Total	C	N	O	P	0	0	0
			349	163	68	101	17			

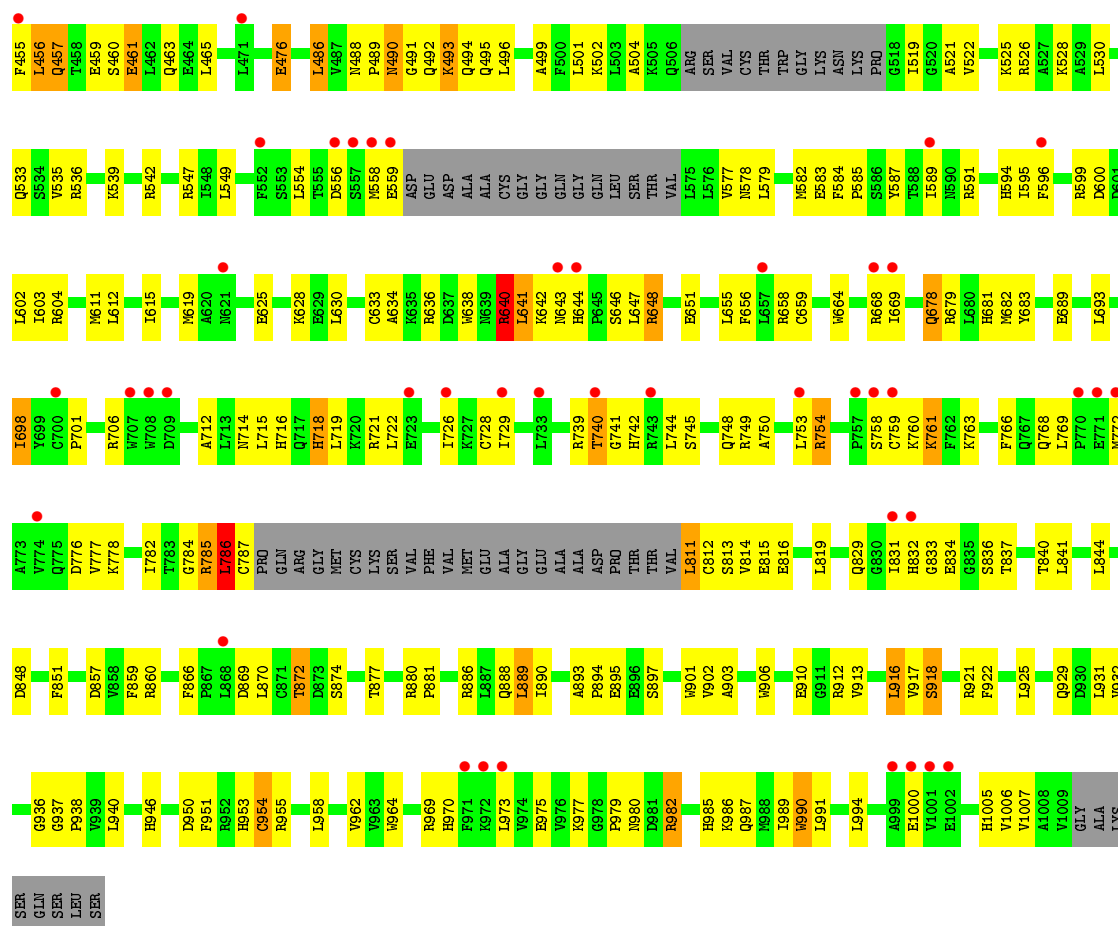
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

- Chain B:

4% 51% 34% 6% 9%

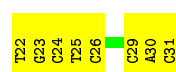
Index	Amino Acid	Chemical Class
1	L916	Polar
2	T837	Positively charged
3	L925	Polar
4	F838	Aromatic
5	S839	Polar
6	T840	Polar
7	L941	Polar
8	L944	Polar
9	D848	Negatively charged
10	M852	Polar
11	L946	Polar
12	L947	Polar
13	D950	Negatively charged
14	F951	Aromatic
15	R952	Positively charged
16	R953	Positively charged
17	G954	Polar
18	R955	Positively charged
19	L958	Polar
20	P959	Polar
21	V962	Polar
22	T872	Polar
23	D873	Negatively charged
24	S874	Polar
25	F875	Aromatic
26	F876	Aromatic
27	T877	Polar
28	R880	Positively charged
29	P881	Polar
30	E884	Negatively charged
31	A885	Polar
32	R886	Positively charged
33	L889	Polar
34	I890	Nonpolar
35	H891	Positively charged
36	P894	Polar
37	E895	Negatively charged
38	C1004	Positively charged
39	H1005	Positively charged
40	V1006	Polar
41	V1007	Polar
42	A1008	Polar
43	G1009	Polar
44	ALA	Polar
45	LYS	Polar
46	SER	Polar
47	GLN	Polar
48	LEU	Polar
49	R912	Positively charged
50	V913	Polar
51	L769	Polar
52	F770	Polar
53	L694	Positively charged
54	L698	Polar
55	S703	Polar
56	R706	Positively charged
57	V707	Polar
58	T781	Polar
59	T782	Polar
60	T783	Polar
61	GLY	Polar
62	ARG	Polar
63	LEU	Polar
64	CYS	Polar
65	PRO	Polar
66	GLN	Polar
67	ARG	Polar
68	GLY	Polar
69	MET	Polar
70	CYS	Polar
71	LYS	Polar
72	SER	Polar
73	D874	Negatively charged
74	PHE	Aromatic
75	VAL	Polar
76	VAL	Polar
77	MET	Polar
78	GLU	Polar
79	ALA	Polar
80	GLU	Polar
81	ALA	Polar
82	ASP	Polar
83	PRO	Polar
84	THR	Polar
85	VAL	Polar
86	C812	Polar
87	S813	Polar
88	B814	Polar
89	E896	Negatively charged
90	S897	Polar
91	E1006	Negatively charged
92	R899	Polar
93	A900	Polar
94	H901	Positively charged
95	V902	Polar
96	A903	Polar
97	W906	Positively charged
98	E910	Negatively charged
99	G911	Polar
100	SER	Polar

- Chain A: 



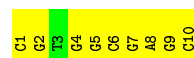
- Molecule 2: DNA (5'-D(*TP*GP*CP*TP*CP*GP*CP*CP*AP*C)-3')

Chain C: 20% 80%



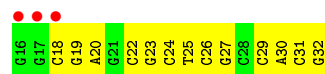
- Molecule 3: DNA (5'-D(P*CP*GP*TP*GP*GP*CP*GP*AP*GP*C)-3')

Chain D: 10% 90%



- Molecule 4: DNA (5'-D(P*GP*GP*CP*GP*AP*GP*CP*GP*CP*TP*CP*GP*CP*CP*AP*C P*G)-3')

Chain E: 18% 24% 76%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	100.96Å 100.96Å 115.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.48 – 3.81 50.48 – 3.81	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.48-3.81) 97.7 (50.48-3.81)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.243 , 0.277 0.273 , 0.301	Depositor DCC
R_{free} test set	614 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	177.6	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 149.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.207 for -h,-k,l 0.349 for h,-h-k,-l 0.218 for -k,-h,-l	Xtriage
Reported twinning fraction	0.490 for H, K, L 0.510 for K, H, -L	Depositor
Outliers	0 of 12619 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10270	wwPDB-VP
Average B, all atoms (Å ²)	221.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% 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	0.55	0/4864	0.80	4/6574 (0.1%)
1	B	0.56	0/4852	0.83	2/6559 (0.0%)
2	C	0.33	0/219	0.74	0/335
3	D	0.57	0/233	0.75	0/358
4	E	0.43	0/391	0.72	0/601
All	All	0.55	0/10559	0.81	6/14427 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	387	LEU	CA-CB-CG	6.77	130.87	115.30
1	A	889	LEU	CA-CB-CG	6.58	130.43	115.30
1	B	693	LEU	CA-CB-CG	6.26	129.70	115.30
1	A	549	LEU	CA-CB-CG	6.04	129.20	115.30
1	A	630	LEU	CA-CB-CG	-5.48	102.69	115.30
1	A	640	ARG	NE-CZ-NH2	-5.23	117.69	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	4764	0	4787	296	0
1	B	4752	0	4761	308	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	197	0	114	10	0
3	D	208	0	112	28	0
4	E	349	0	189	29	0
All	All	10270	0	9963	613	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 31.

All (613) 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:B:813:SER:CB	1:B:816:GLU:HB2	1.17	1.57
1:B:410:LEU:HD11	1:B:414:GLY:C	1.35	1.47
1:B:813:SER:HB3	1:B:816:GLU:CB	1.51	1.38
1:B:813:SER:CB	1:B:816:GLU:CB	2.07	1.29
1:B:781:THR:HG21	1:A:521:ALA:CB	1.66	1.25
1:B:815:GLU:HG3	1:B:832:HIS:CD2	1.73	1.22
1:B:781:THR:HG21	1:A:521:ALA:HB3	1.21	1.18
1:B:642:LYS:O	1:B:647:LEU:CD1	1.92	1.17
1:B:813:SER:OG	1:B:816:GLU:N	1.77	1.16
1:B:946:HIS:HB3	1:B:954:CYS:SG	1.88	1.13
1:A:813:SER:OG	1:A:816:GLU:HG2	1.44	1.13
1:B:410:LEU:CD1	1:B:414:GLY:C	2.17	1.12
1:B:642:LYS:O	1:B:647:LEU:HD12	1.51	1.11
1:B:405:THR:O	1:B:409:GLN:CD	1.85	1.10
1:A:954:CYS:SG	1:A:990:TRP:HZ2	1.76	1.09
1:B:410:LEU:HD22	1:B:411:SER:H	1.17	1.09
1:B:813:SER:OG	1:B:816:GLU:CB	2.01	1.08
1:B:813:SER:OG	1:B:816:GLU:HB2	1.53	1.08
1:A:815:GLU:HG3	1:A:832:HIS:NE2	1.69	1.06
1:B:410:LEU:HD11	1:B:414:GLY:CA	1.84	1.06
1:A:950:ASP:OD2	1:A:953:HIS:HD2	1.40	1.05
1:A:813:SER:OG	1:A:816:GLU:CG	2.05	1.03
1:A:815:GLU:HB3	1:A:832:HIS:HD2	1.20	1.03
1:B:715:LEU:HD12	1:B:715:LEU:H	1.19	1.02
1:A:950:ASP:OD2	1:A:953:HIS:CD2	2.13	1.01
1:B:473:SER:HB2	4:E:20:DA:OP2	1.56	1.01
3:D:1:DC:N3	4:E:32:DG:O6	1.93	1.01
3:D:7:DG:N2	4:E:26:DC:N3	2.06	1.00
1:A:390:GLU:HG3	4:E:32:DG:H5"	1.42	1.00
1:B:474:ALA:HA	1:B:493:LYS:HD2	1.41	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:10:DC:O2	4:E:23:DG:N2	1.94	0.99
1:A:815:GLU:HB3	1:A:832:HIS:CD2	1.98	0.98
1:A:894:PRO:HG2	1:A:897:SER:OG	1.63	0.98
1:A:894:PRO:CG	1:A:897:SER:OG	2.12	0.98
1:A:785:ARG:HB3	1:A:786:LEU:HD13	1.46	0.98
1:B:781:THR:HG22	1:B:1005:HIS:HB2	1.46	0.97
1:A:651:GLU:HG2	1:A:698:ILE:HG12	1.47	0.96
1:B:480:LEU:HD11	1:B:526:ARG:HB3	1.46	0.96
1:B:410:LEU:CD1	1:B:415:GLN:N	2.29	0.95
1:B:833:GLY:HA3	1:B:837:THR:OG1	1.66	0.95
1:B:815:GLU:HG3	1:B:832:HIS:NE2	1.82	0.95
1:B:410:LEU:CD2	1:B:449:GLU:CD	2.36	0.94
1:A:813:SER:HG	1:A:816:GLU:HG2	1.24	0.94
1:A:461:GLU:OE1	1:A:461:GLU:O	1.85	0.94
1:A:950:ASP:OD1	1:A:953:HIS:CD2	2.20	0.94
1:A:815:GLU:CB	1:A:832:HIS:CD2	2.50	0.93
3:D:2:DG:N2	4:E:31:DC:O2	2.01	0.93
3:D:7:DG:H1	4:E:26:DC:H42	0.94	0.92
1:A:786:LEU:HD22	1:A:812:CYS:H	1.33	0.92
1:A:719:LEU:HD12	1:A:721:ARG:NH1	1.85	0.92
1:A:786:LEU:HD22	1:A:812:CYS:N	1.85	0.91
1:A:950:ASP:CG	1:A:953:HIS:HD2	1.72	0.91
1:B:410:LEU:HD22	1:B:411:SER:N	1.85	0.90
3:D:7:DG:H1	4:E:26:DC:N4	1.68	0.90
1:A:950:ASP:CG	1:A:953:HIS:CD2	2.47	0.88
1:B:739:ARG:CB	1:B:953:HIS:CD2	2.56	0.88
1:B:815:GLU:CG	1:B:832:HIS:CD2	2.56	0.87
1:A:815:GLU:CG	1:A:832:HIS:NE2	2.37	0.86
1:B:703:SER:HB2	1:B:707:TRP:CZ2	2.10	0.86
1:B:583:GLU:O	1:B:912:ARG:HA	1.76	0.85
1:A:644:HIS:CE1	1:A:646:SER:OG	2.29	0.85
1:A:390:GLU:HG3	4:E:32:DG:C5'	2.06	0.84
1:B:950:ASP:OD1	1:B:953:HIS:CD2	2.30	0.84
1:B:715:LEU:HA	1:B:719:LEU:HB2	1.58	0.84
1:A:493:LYS:H	1:A:493:LYS:HE2	1.43	0.84
1:B:781:THR:HG21	1:A:521:ALA:HB1	1.59	0.84
1:B:739:ARG:CB	1:B:953:HIS:NE2	2.42	0.83
1:A:493:LYS:H	1:A:493:LYS:CE	1.92	0.83
1:A:813:SER:HG	1:A:816:GLU:CG	1.88	0.83
1:B:410:LEU:HD21	1:B:449:GLU:OE1	1.78	0.83
1:B:813:SER:OG	1:B:816:GLU:CA	2.27	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:LEU:HD12	1:A:584:PHE:HZ	1.44	0.82
1:B:822:TYR:CE2	1:B:974:VAL:HG21	2.15	0.82
1:B:727:LYS:O	1:B:731:GLU:HG3	1.79	0.82
1:A:644:HIS:CE1	1:A:646:SER:H	1.98	0.81
1:A:832:HIS:ND1	1:A:832:HIS:O	2.11	0.81
3:D:2:DG:N1	4:E:31:DC:N3	2.28	0.81
1:B:481:ALA:HA	1:B:500:PHE:HZ	1.45	0.81
3:D:9:DG:N2	4:E:24:DC:O2	2.14	0.81
1:B:950:ASP:OD1	1:B:953:HIS:HD2	1.62	0.80
1:B:410:LEU:CD2	1:B:449:GLU:OE1	2.30	0.79
1:B:781:THR:CG2	1:A:521:ALA:HB3	2.09	0.79
1:A:754:ARG:O	1:A:754:ARG:HG3	1.80	0.79
1:B:832:HIS:O	1:B:832:HIS:ND1	2.16	0.79
1:B:387:LEU:HA	1:B:393:MET:SD	2.23	0.79
1:B:410:LEU:HD11	1:B:414:GLY:HA3	1.65	0.78
1:B:815:GLU:HG3	1:B:832:HIS:HD2	1.45	0.78
1:B:813:SER:HG	1:B:816:GLU:H	1.29	0.78
1:A:877:THR:HG22	1:A:880:ARG:HH21	1.47	0.78
1:B:430:LYS:HB2	1:B:433:LYS:HG2	1.64	0.78
1:B:714:ASN:O	1:B:717:GLN:O	2.02	0.78
1:B:583:GLU:HB3	1:B:912:ARG:HE	1.48	0.78
1:A:870:LEU:HD21	1:A:916:LEU:HD21	1.66	0.77
1:B:1005:HIS:HB3	1:A:525:LYS:NZ	1.98	0.77
1:A:786:LEU:HD21	1:A:812:CYS:SG	2.25	0.77
1:B:706:ARG:HA	1:B:742:HIS:CE1	2.19	0.77
1:B:1005:HIS:HD2	1:A:525:LYS:HE2	1.50	0.76
1:B:946:HIS:CB	1:B:954:CYS:SG	2.72	0.76
1:B:405:THR:O	1:B:409:GLN:NE2	2.18	0.76
1:A:815:GLU:CG	1:A:832:HIS:CD2	2.68	0.75
1:B:409:GLN:NE2	1:B:409:GLN:H	1.84	0.75
1:A:644:HIS:CE1	1:A:646:SER:CB	2.69	0.75
1:A:716:HIS:ND1	1:A:753:LEU:HD21	2.00	0.75
1:A:579:LEU:HD12	1:A:584:PHE:CZ	2.21	0.75
1:B:813:SER:CB	1:B:816:GLU:CG	2.64	0.74
1:B:916:LEU:CD2	1:B:951:PHE:CE2	2.69	0.74
1:B:481:ALA:HA	1:B:500:PHE:CZ	2.22	0.74
1:A:754:ARG:HH11	1:A:766:PHE:HB2	1.49	0.74
1:B:813:SER:O	1:B:817:LEU:N	2.18	0.74
1:A:918:SER:HB2	1:A:921:ARG:HB2	1.70	0.74
1:B:659:CYS:HA	1:B:664:TRP:CD2	2.23	0.74
1:B:779:HIS:HB2	1:A:522:VAL:CG2	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:815:GLU:CG	1:B:832:HIS:HD2	1.99	0.73
1:A:644:HIS:HE1	1:A:646:SER:HB3	1.54	0.72
1:B:954:CYS:HG	1:B:990:TRP:HZ2	1.36	0.72
1:A:401:LYS:CE	3:D:5:DG:OP1	2.37	0.72
1:B:631:ALA:HB1	1:B:673:PHE:HD1	1.54	0.72
1:B:954:CYS:SG	1:B:990:TRP:HZ2	2.12	0.72
1:A:785:ARG:HB3	1:A:786:LEU:CD1	2.19	0.71
1:B:813:SER:HB3	1:B:816:GLU:HB2	0.72	0.71
1:A:872:THR:HG23	1:A:874:SER:H	1.54	0.71
1:B:410:LEU:HD23	1:B:449:GLU:CD	2.09	0.71
3:D:1:DC:N3	4:E:32:DG:C6	2.57	0.71
1:B:779:HIS:HB2	1:A:522:VAL:HG21	1.73	0.71
1:A:644:HIS:HE1	1:A:646:SER:CB	2.02	0.70
1:A:754:ARG:NH1	1:A:766:PHE:HB2	2.07	0.70
1:A:740:THR:HB	1:A:989:ILE:HG21	1.73	0.70
1:A:655:LEU:HD23	1:A:658:ARG:HH21	1.55	0.70
1:A:895:GLU:OE2	1:A:969:ARG:NH1	2.24	0.70
1:B:1005:HIS:CD2	1:A:525:LYS:HE2	2.27	0.70
1:A:579:LEU:CD1	1:A:584:PHE:CZ	2.75	0.69
1:A:376:LEU:HD22	1:A:380:LEU:HD11	1.73	0.69
1:A:426:LEU:HD13	1:A:542:ARG:HD2	1.73	0.69
1:B:834:GLU:N	1:B:834:GLU:OE1	2.25	0.69
1:A:600:ASP:HB3	1:A:604:ARG:HH12	1.58	0.69
1:B:616:SER:HA	1:B:619:MET:HE2	1.75	0.68
1:B:903:ALA:HA	1:B:925:LEU:HD11	1.75	0.68
1:A:504:ALA:HA	1:A:519:ILE:HG23	1.76	0.68
1:B:744:LEU:HB2	1:B:989:ILE:HD11	1.76	0.68
1:A:813:SER:OG	1:A:816:GLU:HG3	1.93	0.68
1:A:493:LYS:H	1:A:493:LYS:NZ	1.92	0.68
1:B:410:LEU:CD1	1:B:414:GLY:CA	2.67	0.68
1:B:410:LEU:HD13	1:B:411:SER:O	1.94	0.68
1:B:410:LEU:HD22	1:B:449:GLU:OE2	1.93	0.68
1:B:667:THR:HG23	1:B:693:LEU:HD22	1.76	0.68
1:A:461:GLU:OE1	1:A:463:GLN:HG2	1.94	0.67
1:B:653:LEU:O	1:B:658:ARG:NH1	2.27	0.67
1:A:401:LYS:HG2	3:D:4:DG:H3'	1.76	0.67
1:A:493:LYS:HZ3	1:A:493:LYS:N	1.92	0.67
1:A:659:CYS:HA	1:A:664:TRP:CD2	2.29	0.67
1:A:689:GLU:O	1:A:693:LEU:HG	1.93	0.67
1:B:410:LEU:HD11	1:B:414:GLY:O	1.91	0.67
1:A:954:CYS:SG	1:A:990:TRP:CZ2	2.64	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:869:ASP:O	1:B:872:THR:HG22	1.95	0.67
1:B:1005:HIS:HB3	1:A:525:LYS:HZ1	1.56	0.67
3:D:2:DG:O6	4:E:30:DA:N1	2.28	0.67
1:A:461:GLU:C	1:A:461:GLU:OE1	2.33	0.67
1:A:729:ILE:HG21	1:A:750:ALA:HB2	1.77	0.66
1:B:642:LYS:O	1:B:647:LEU:HD11	1.90	0.66
1:B:916:LEU:HD23	1:B:951:PHE:CE2	2.28	0.66
1:B:668:ARG:O	1:B:672:ARG:HG2	1.96	0.66
1:B:815:GLU:HB3	1:B:832:HIS:HD2	1.58	0.66
1:B:715:LEU:N	1:B:715:LEU:HD12	2.03	0.66
1:B:815:GLU:CB	1:B:832:HIS:HD2	2.08	0.66
1:B:954:CYS:HA	1:B:990:TRP:CZ2	2.31	0.66
1:B:410:LEU:CD1	1:B:414:GLY:HA3	2.25	0.66
1:B:658:ARG:HH11	1:B:658:ARG:HG3	1.61	0.65
1:B:837:THR:HG21	1:B:962:VAL:HG11	1.77	0.65
1:B:714:ASN:ND2	1:B:714:ASN:H	1.92	0.65
1:B:631:ALA:HB1	1:B:673:PHE:CD1	2.31	0.65
1:B:687:VAL:HG13	1:B:711:LEU:HD11	1.79	0.65
1:B:673:PHE:HA	1:B:676:ILE:HD12	1.79	0.65
1:A:644:HIS:CE1	1:A:646:SER:HG	2.13	0.65
1:A:894:PRO:HG2	1:A:897:SER:CB	2.27	0.65
1:B:410:LEU:CD2	1:B:449:GLU:OE2	2.43	0.65
1:B:389:ASN:O	1:B:393:MET:HG2	1.97	0.65
1:A:829:GLN:HB2	1:A:964:TRP:CE2	2.32	0.64
1:B:717:GLN:HB3	1:B:718:HIS:CD2	2.31	0.64
1:B:590:ASN:ND2	1:B:856:PRO:HA	2.11	0.64
1:A:719:LEU:HD12	1:A:721:ARG:HH11	1.60	0.64
1:B:950:ASP:OD2	1:B:953:HIS:HB2	1.97	0.63
1:B:955:ARG:HH11	1:B:955:ARG:CG	2.11	0.63
1:B:477:LEU:HD21	1:B:497:VAL:HG23	1.80	0.63
1:A:401:LYS:HE2	3:D:5:DG:OP1	1.98	0.63
3:D:8:DA:N1	4:E:25:DT:O4	2.32	0.63
3:D:1:DC:C4	4:E:32:DG:O6	2.50	0.63
1:A:815:GLU:HG3	1:A:832:HIS:CD2	2.31	0.63
1:A:840:THR:HG21	1:A:922:PHE:HE2	1.63	0.63
1:A:833:GLY:O	1:A:836:SER:OG	2.16	0.63
1:B:813:SER:CB	1:B:816:GLU:HG3	2.29	0.63
1:A:493:LYS:HB3	1:A:493:LYS:NZ	2.13	0.62
1:B:424:ARG:HG2	2:C:30:DA:H5"	1.81	0.62
1:B:821:HIS:HA	1:B:824:ARG:HE	1.64	0.62
1:A:493:LYS:H	1:A:493:LYS:HZ3	1.45	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:716:HIS:CD2	1:B:753:LEU:HD21	2.33	0.62
3:D:2:DG:O6	4:E:30:DA:C6	2.53	0.62
1:B:954:CYS:SG	1:B:990:TRP:CZ2	2.91	0.62
1:B:715:LEU:CD1	1:B:715:LEU:H	2.01	0.62
1:A:889:LEU:O	1:A:893:ALA:HB2	1.99	0.62
1:A:486:LEU:O	1:A:489:PRO:HG3	2.00	0.62
1:B:916:LEU:CD2	1:B:951:PHE:HE2	2.13	0.62
1:B:694:LEU:HD23	1:B:707:TRP:HE3	1.64	0.61
1:B:723:GLU:O	1:B:727:LYS:HG3	1.99	0.61
1:A:393:MET:HA	1:A:393:MET:CE	2.31	0.61
1:B:386:VAL:HG12	1:B:393:MET:HE1	1.83	0.61
1:A:547:ARG:HB3	1:A:602:LEU:HD21	1.82	0.60
1:A:894:PRO:CD	1:A:897:SER:OG	2.49	0.60
1:A:584:PHE:O	1:A:912:ARG:HD2	2.00	0.60
1:A:585:PRO:HD3	1:A:913:VAL:O	2.02	0.60
1:B:1005:HIS:CD2	1:A:525:LYS:HG2	2.37	0.60
1:A:946:HIS:HB3	1:A:954:CYS:SG	2.41	0.60
1:B:723:GLU:HB3	1:B:724:PRO:HD3	1.84	0.60
1:B:729:ILE:HG21	1:B:750:ALA:HB2	1.83	0.60
1:B:694:LEU:HD21	1:B:707:TRP:HB2	1.83	0.60
1:A:604:ARG:NH2	1:A:644:HIS:NE2	2.50	0.59
1:B:744:LEU:HD22	1:B:989:ILE:HG12	1.83	0.59
3:D:1:DC:O2	4:E:32:DG:N1	2.30	0.59
1:A:659:CYS:HA	1:A:664:TRP:CG	2.37	0.59
1:B:552:PHE:HE2	1:B:575:LEU:N	2.00	0.59
1:A:547:ARG:HD2	1:A:602:LEU:HG	1.84	0.59
1:A:644:HIS:CE1	1:A:646:SER:N	2.70	0.59
1:A:816:GLU:HA	1:A:819:LEU:HD12	1.85	0.59
1:A:461:GLU:CA	1:A:461:GLU:OE1	2.51	0.59
1:A:716:HIS:CE1	1:A:753:LEU:HG	2.38	0.59
1:B:372:PHE:HZ	1:B:380:LEU:HD12	1.68	0.59
1:A:611:MET:SD	1:A:634:ALA:HB2	2.43	0.59
1:B:410:LEU:HD21	1:B:414:GLY:HA3	1.83	0.59
1:B:680:LEU:HD22	1:A:441:LEU:HD13	1.85	0.59
1:B:436:TYR:HE1	2:C:31:DC:OP1	1.86	0.59
1:A:786:LEU:CD2	1:A:812:CYS:SG	2.90	0.59
1:B:977:LYS:HB2	1:B:1005:HIS:CD2	2.37	0.59
1:B:377:ARG:HG2	1:B:580:GLY:HA3	1.85	0.59
1:A:714:ASN:O	1:A:719:LEU:HD23	2.03	0.59
1:A:754:ARG:HD3	1:A:766:PHE:CG	2.37	0.59
1:A:786:LEU:HB2	1:A:811:LEU:HA	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:814:VAL:HG23	1:B:815:GLU:N	2.18	0.59
1:B:424:ARG:CZ	2:C:30:DA:H5''	2.32	0.58
1:B:872:THR:HG23	1:B:874:SER:H	1.68	0.58
1:A:579:LEU:CD1	1:A:584:PHE:HZ	2.13	0.58
3:D:8:DA:N1	4:E:25:DT:C4	2.72	0.58
1:B:715:LEU:O	1:B:720:LYS:N	2.36	0.58
1:B:384:LYS:HD2	1:B:385:THR:N	2.17	0.58
1:A:398:GLU:CD	3:D:4:DG:OP2	2.42	0.58
4:E:31:DC:H1'	4:E:32:DG:C8	2.39	0.57
1:A:374:TYR:CE2	1:A:577:VAL:HG13	2.39	0.57
1:A:456:LEU:HD23	1:A:536:ARG:O	2.03	0.57
1:B:820:ALA:O	1:B:824:ARG:HG3	2.04	0.57
1:B:583:GLU:HB3	1:B:912:ARG:NE	2.17	0.57
1:A:840:THR:HG23	1:A:917:VAL:HG13	1.86	0.57
1:B:955:ARG:NH1	1:B:955:ARG:HG3	2.19	0.57
1:A:656:PHE:CB	1:A:869:ASP:HA	2.35	0.57
1:B:644:HIS:HE1	1:B:646:SER:HB3	1.70	0.56
1:B:813:SER:OG	1:B:816:GLU:CG	2.52	0.56
1:B:952:ARG:HB2	1:B:952:ARG:CZ	2.35	0.56
1:A:490:ASN:OD1	1:A:490:ASN:N	2.39	0.56
1:A:492:GLN:O	1:A:495:GLN:HG2	2.04	0.56
1:A:745:SER:HB2	1:A:985:HIS:CD2	2.40	0.56
1:B:424:ARG:HG2	2:C:30:DA:C5'	2.35	0.56
1:B:783:THR:HA	1:B:1007:VAL:HG22	1.86	0.56
1:A:784:GLY:N	1:A:1007:VAL:O	2.38	0.56
1:B:597:GLN:HG3	1:B:649:CYS:HB2	1.87	0.56
1:B:952:ARG:HB3	1:B:952:ARG:NH1	2.20	0.56
1:A:954:CYS:HA	1:A:990:TRP:CZ2	2.40	0.56
1:A:716:HIS:CE1	1:A:753:LEU:CD2	2.89	0.56
1:B:755:GLU:O	1:B:755:GLU:HG2	2.06	0.56
1:B:980:ASN:HD21	1:A:460:SER:HB2	1.70	0.56
1:B:815:GLU:HA	1:B:815:GLU:OE1	2.06	0.56
1:B:583:GLU:CB	1:B:912:ARG:HE	2.17	0.56
4:E:29:DC:H2''	4:E:30:DA:C8	2.41	0.56
1:A:840:THR:CG2	1:A:922:PHE:HE2	2.20	0.56
1:B:405:THR:O	1:B:409:GLN:CG	2.54	0.56
1:B:744:LEU:HD23	1:B:985:HIS:HB3	1.88	0.56
1:A:848:ASP:OD1	1:A:886:ARG:NH2	2.36	0.55
1:B:492:GLN:O	1:B:495:GLN:HG2	2.06	0.55
1:B:616:SER:HA	1:B:619:MET:CE	2.35	0.55
1:A:880:ARG:N	1:A:881:PRO:HD2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:LYS:O	1:A:647:LEU:HD12	2.06	0.55
1:B:712:ALA:HA	1:B:715:LEU:HD13	1.88	0.55
1:B:815:GLU:CB	1:B:832:HIS:CD2	2.88	0.55
1:B:903:ALA:HA	1:B:925:LEU:CD1	2.36	0.55
1:B:411:SER:HG	1:B:449:GLU:CD	2.09	0.55
1:A:579:LEU:HD13	1:A:582:MET:CE	2.37	0.55
1:A:714:ASN:HA	1:A:718:HIS:HB2	1.89	0.55
1:A:840:THR:HG21	1:A:922:PHE:CE2	2.41	0.55
1:A:950:ASP:O	1:A:954:CYS:HB2	2.07	0.55
1:B:666:TYR:O	1:B:670:LEU:HG	2.07	0.55
1:A:636:ARG:HB2	1:A:636:ARG:NH1	2.22	0.54
1:B:838:PHE:HA	1:B:841:LEU:HD12	1.89	0.54
1:A:376:LEU:HD22	1:A:380:LEU:CD1	2.36	0.54
1:B:430:LYS:NZ	1:B:476:GLU:OE1	2.39	0.54
1:A:579:LEU:CD1	1:A:584:PHE:CE2	2.90	0.54
1:A:615:ILE:HG22	1:A:619:MET:HE2	1.90	0.54
1:A:656:PHE:HB2	1:A:869:ASP:HA	1.89	0.54
1:A:866:PHE:HB2	1:A:870:LEU:HD22	1.89	0.54
1:A:640:ARG:HH11	1:A:640:ARG:HA	1.73	0.54
1:A:395:LEU:O	1:A:599:ARG:HA	2.07	0.54
1:B:897:SER:HB3	1:B:901:TRP:CZ2	2.43	0.54
1:A:391:ASP:HA	1:A:394:LEU:HD12	1.90	0.54
1:A:831:ILE:HG21	1:A:921:ARG:HD2	1.89	0.54
1:A:833:GLY:HA3	1:A:921:ARG:NE	2.23	0.54
1:B:644:HIS:CG	1:B:645:PRO:HD2	2.43	0.54
1:B:880:ARG:O	1:B:884:GLU:HG2	2.08	0.54
1:A:844:LEU:HD13	1:A:902:VAL:HG13	1.88	0.53
1:B:430:LYS:HG3	1:B:471:LEU:HD11	1.91	0.53
1:B:410:LEU:CD2	1:B:414:GLY:HA3	2.39	0.53
3:D:7:DG:N2	4:E:26:DC:C2	2.65	0.53
1:A:604:ARG:NH2	1:A:644:HIS:CE1	2.76	0.53
1:A:760:LYS:O	1:A:763:LYS:HD2	2.08	0.53
1:B:481:ALA:CA	1:B:500:PHE:HZ	2.19	0.53
1:B:947:LEU:HD23	1:B:954:CYS:HB3	1.89	0.53
1:A:406:LYS:HG3	1:A:455:PHE:HE2	1.74	0.53
1:A:640:ARG:O	1:A:640:ARG:CZ	2.57	0.53
1:B:410:LEU:HD22	1:B:449:GLU:CD	2.27	0.53
1:B:465:LEU:HD21	1:B:520:GLY:HA2	1.89	0.53
1:B:706:ARG:HH11	1:B:706:ARG:CB	2.22	0.53
1:B:722:LEU:O	1:B:726:ILE:HG12	2.09	0.53
1:B:858:VAL:HG23	1:B:859:PHE:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:MET:HE3	1:B:533:GLN:HB3	1.90	0.53
1:B:582:MET:HG3	1:B:584:PHE:CE1	2.44	0.53
1:A:648:ARG:HB3	1:A:648:ARG:CZ	2.38	0.53
1:A:715:LEU:HA	1:A:719:LEU:HB2	1.90	0.53
1:B:694:LEU:CD2	1:B:707:TRP:HE3	2.22	0.53
1:B:838:PHE:HB2	1:B:958:LEU:HD13	1.90	0.53
1:A:416:LYS:HD2	1:A:439:ILE:HG12	1.90	0.53
1:A:493:LYS:HG2	1:A:494:GLN:N	2.24	0.53
1:A:831:ILE:CG2	1:A:921:ARG:HD2	2.39	0.53
1:B:638:TRP:HB2	1:B:666:TYR:CG	2.44	0.52
1:B:688:ARG:HH11	1:B:689:GLU:HG2	1.73	0.52
1:B:395:LEU:HB3	1:B:602:LEU:HD22	1.90	0.52
1:A:894:PRO:HD2	1:A:897:SER:OG	2.08	0.52
1:A:716:HIS:CE1	1:A:753:LEU:HD21	2.45	0.52
1:A:754:ARG:HD3	1:A:766:PHE:CB	2.39	0.52
1:B:955:ARG:NH1	1:B:955:ARG:CG	2.71	0.52
1:A:387:LEU:CD1	1:A:401:LYS:NZ	2.73	0.52
1:B:409:GLN:N	1:B:409:GLN:NE2	2.55	0.52
1:B:411:SER:OG	1:B:449:GLU:OE2	2.27	0.52
1:B:813:SER:HB3	1:B:816:GLU:CG	2.32	0.52
1:A:486:LEU:HD21	1:A:499:ALA:HB1	1.91	0.52
1:A:837:THR:O	1:A:841:LEU:HD12	2.10	0.52
1:A:931:LEU:HD11	1:A:962:VAL:HG21	1.91	0.52
1:A:383:LEU:O	1:A:387:LEU:HD23	2.10	0.51
1:A:716:HIS:ND1	1:A:753:LEU:CD2	2.70	0.51
1:A:903:ALA:HB2	1:A:929:GLN:NE2	2.25	0.51
1:B:718:HIS:N	1:B:718:HIS:CD2	2.77	0.51
1:B:779:HIS:CB	1:A:522:VAL:HG22	2.40	0.51
1:B:916:LEU:HD23	1:B:951:PHE:CZ	2.46	0.51
1:B:411:SER:O	1:B:415:GLN:N	2.43	0.51
1:B:625:GLU:O	1:B:629:GLU:HG2	2.09	0.51
1:A:712:ALA:HB1	1:A:749:ARG:HD2	1.91	0.51
1:B:779:HIS:HB2	1:A:522:VAL:HG22	1.93	0.51
1:A:461:GLU:OE1	1:A:461:GLU:HA	2.11	0.51
1:A:987:GLN:O	1:A:991:LEU:HG	2.10	0.51
1:B:955:ARG:HG3	1:B:955:ARG:HH11	1.75	0.51
1:A:491:GLY:O	1:A:496:LEU:HG	2.10	0.51
1:B:436:TYR:CE1	2:C:31:DC:OP1	2.63	0.51
1:B:582:MET:HG3	1:B:584:PHE:HE1	1.75	0.51
1:A:633:CYS:HA	1:A:636:ARG:NH1	2.25	0.51
1:B:706:ARG:HH11	1:B:706:ARG:HB3	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1005:HIS:HB3	1:A:525:LYS:HZ3	1.76	0.50
1:B:690:LEU:HD13	1:B:711:LEU:HB2	1.92	0.50
1:B:590:ASN:N	1:B:859:PHE:O	2.44	0.50
1:A:829:GLN:HB2	1:A:964:TRP:CD2	2.47	0.50
1:A:456:LEU:CD2	1:A:535:VAL:HB	2.41	0.50
1:B:952:ARG:CB	1:B:952:ARG:CZ	2.89	0.50
1:A:754:ARG:O	1:A:754:ARG:CG	2.55	0.50
1:A:814:VAL:HG23	1:A:815:GLU:N	2.26	0.50
1:A:476:GLU:OE1	1:A:476:GLU:HA	2.12	0.50
1:A:785:ARG:O	1:A:786:LEU:HB2	2.12	0.50
1:A:387:LEU:CD1	1:A:401:LYS:HZ1	2.25	0.50
1:B:779:HIS:CD2	1:A:522:VAL:HG13	2.47	0.49
1:B:644:HIS:CE1	1:B:646:SER:HB3	2.47	0.49
1:B:380:LEU:HD22	1:B:408:TYR:HE1	1.76	0.49
1:A:834:GLU:OE1	1:A:834:GLU:N	2.45	0.49
1:B:815:GLU:HB3	1:B:832:HIS:CD2	2.43	0.49
1:B:403:ILE:HA	1:B:406:LYS:HE2	1.93	0.49
1:B:416:LYS:HB3	1:B:439:ILE:HG12	1.94	0.49
1:A:401:LYS:NZ	3:D:5:DG:OP1	2.46	0.49
1:A:591:ARG:HE	1:A:860:ARG:HB3	1.77	0.49
1:B:463:GLN:HA	1:B:524:LEU:HD21	1.93	0.49
1:B:587:TYR:CD1	1:B:859:PHE:HB3	2.47	0.49
1:B:762:PHE:HB3	1:B:765:LEU:HD12	1.94	0.49
1:B:670:LEU:HB2	1:B:693:LEU:HD21	1.93	0.49
1:A:888:GLN:HA	1:A:888:GLN:OE1	2.12	0.49
1:B:378:SER:OG	1:B:575:LEU:O	2.28	0.49
1:B:703:SER:HB2	1:B:707:TRP:CE2	2.46	0.49
1:B:886:ARG:HD3	1:B:889:LEU:HD23	1.95	0.49
1:A:951:PHE:CZ	1:A:955:ARG:HD2	2.48	0.49
1:A:744:LEU:HB2	1:A:989:ILE:HD11	1.94	0.49
1:B:947:LEU:O	1:B:951:PHE:HB2	2.12	0.49
1:B:894:PRO:HD2	1:B:897:SER:OG	2.13	0.49
1:B:706:ARG:HA	1:B:742:HIS:ND1	2.26	0.48
1:A:428:TRP:O	1:A:429:ILE:HG13	2.14	0.48
1:B:717:GLN:C	1:B:718:HIS:CD2	2.85	0.48
1:B:760:LYS:HG3	1:B:761:LYS:N	2.28	0.48
3:D:8:DA:H2	4:E:25:DT:H3	1.54	0.48
1:A:387:LEU:HD11	1:A:401:LYS:HZ1	1.78	0.48
1:A:681:HIS:HA	1:A:683:TYR:CZ	2.47	0.48
1:B:382:VAL:O	1:B:386:VAL:HG23	2.14	0.48
1:B:631:ALA:CB	1:B:673:PHE:HD1	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:25:DT:H2"	2:C:26:DC:O5'	2.13	0.48
1:A:488:ASN:N	1:A:489:PRO:HD3	2.29	0.48
1:A:722:LEU:O	1:A:726:ILE:HG12	2.14	0.48
1:B:814:VAL:CG2	1:B:815:GLU:N	2.76	0.48
1:A:493:LYS:HZ3	1:A:493:LYS:HB3	1.76	0.48
1:A:633:CYS:HA	1:A:636:ARG:HH12	1.78	0.48
1:A:741:GLY:O	1:A:985:HIS:HB2	2.12	0.48
1:A:786:LEU:N	1:A:786:LEU:HD12	2.28	0.48
1:A:982:ARG:HD3	1:A:982:ARG:N	2.29	0.48
1:B:673:PHE:O	1:B:677:LEU:HG	2.12	0.48
1:A:894:PRO:HD2	1:A:897:SER:CB	2.44	0.48
1:B:952:ARG:HB3	1:B:952:ARG:HH11	1.78	0.48
1:B:952:ARG:CB	1:B:952:ARG:NH1	2.76	0.48
1:A:636:ARG:CB	1:A:636:ARG:HH11	2.27	0.47
1:A:638:TRP:O	1:A:642:LYS:HG3	2.14	0.47
1:A:644:HIS:CE1	1:A:646:SER:HB3	2.39	0.47
1:B:492:GLN:HA	1:B:492:GLN:OE1	2.12	0.47
1:B:592:LYS:HB2	1:B:857:ASP:OD2	2.13	0.47
1:A:857:ASP:OD1	1:A:860:ARG:NH1	2.47	0.47
1:B:424:ARG:NE	2:C:30:DA:H5"	2.29	0.47
1:B:377:ARG:CG	1:B:580:GLY:HA3	2.44	0.47
1:B:410:LEU:HD12	1:B:415:GLN:HA	1.96	0.47
1:B:622:GLY:HA2	1:B:624:TRP:NE1	2.28	0.47
1:B:462:LEU:HD11	1:B:468:VAL:HB	1.97	0.47
1:B:421:LEU:HB2	1:B:537:ILE:HD11	1.97	0.47
1:B:951:PHE:CD1	1:B:951:PHE:C	2.87	0.47
1:A:493:LYS:HG2	1:A:494:GLN:H	1.77	0.47
2:C:24:DC:H2"	2:C:25:DT:H5"	1.97	0.47
1:A:374:TYR:CG	1:A:375:TYR:N	2.82	0.47
1:B:1005:HIS:CD2	1:A:525:LYS:CE	2.96	0.47
1:A:768:GLN:NE2	1:A:769:LEU:HG	2.29	0.47
1:B:980:ASN:H	1:A:528:LYS:NZ	2.13	0.47
1:B:716:HIS:ND1	1:B:749:ARG:NH1	2.62	0.47
1:A:719:LEU:CD2	1:A:719:LEU:N	2.78	0.47
3:D:9:DG:N1	4:E:24:DC:N3	2.60	0.47
1:A:579:LEU:HD13	1:A:582:MET:HE3	1.95	0.47
1:A:777:VAL:HG12	1:A:778:LYS:H	1.80	0.47
1:A:584:PHE:HA	1:A:913:VAL:HG22	1.97	0.47
1:B:744:LEU:HD23	1:B:985:HIS:CB	2.44	0.47
1:B:420:ARG:O	1:B:424:ARG:HG3	2.15	0.47
3:D:1:DC:C2	4:E:32:DG:N1	2.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:LEU:N	1:A:719:LEU:HD22	2.30	0.46
1:B:980:ASN:HD21	1:A:460:SER:CB	2.28	0.46
1:A:604:ARG:HD2	1:A:641:LEU:CD2	2.45	0.46
1:A:973:LEU:HD12	1:A:994:LEU:HD13	1.97	0.46
1:A:406:LYS:HE3	1:A:453:ALA:HB1	1.97	0.46
1:A:851:PHE:HA	1:A:859:PHE:HZ	1.81	0.46
1:B:420:ARG:HG3	1:B:439:ILE:HD11	1.98	0.46
1:B:407:PHE:HB2	1:B:455:PHE:CZ	2.51	0.46
1:B:832:HIS:CE1	1:B:834:GLU:CD	2.89	0.46
1:B:813:SER:HB2	1:B:816:GLU:HG3	1.98	0.46
1:A:950:ASP:OD2	1:A:953:HIS:HB2	2.16	0.46
1:B:378:SER:O	1:B:382:VAL:HG23	2.16	0.46
1:B:393:MET:HB3	1:B:401:LYS:HE2	1.98	0.46
1:A:493:LYS:CB	1:A:493:LYS:NZ	2.79	0.46
1:A:426:LEU:HD21	1:A:539:LYS:HD3	1.97	0.46
1:A:678:GLN:OE1	1:A:714:ASN:ND2	2.49	0.46
1:A:719:LEU:HB3	1:A:721:ARG:HD2	1.98	0.46
1:B:410:LEU:HD13	1:B:415:GLN:N	2.24	0.46
1:B:632:GLN:HB3	1:B:636:ARG:HH12	1.81	0.46
1:A:444:THR:HA	1:A:447:ILE:HD12	1.98	0.45
1:A:903:ALA:HA	1:A:925:LEU:HD11	1.97	0.45
1:A:493:LYS:HE2	1:A:493:LYS:N	2.21	0.45
1:B:407:PHE:O	1:B:410:LEU:HB3	2.17	0.45
1:B:622:GLY:HA2	1:B:624:TRP:HE1	1.81	0.45
1:B:891:HIS:HD1	1:B:891:HIS:C	2.19	0.45
1:A:431:MET:SD	1:A:533:GLN:HB3	2.56	0.45
1:A:489:PRO:O	1:A:496:LEU:HD21	2.17	0.45
1:A:958:LEU:HD23	1:A:990:TRP:HD1	1.81	0.45
1:B:411:SER:OG	1:B:449:GLU:OE1	2.34	0.45
1:B:658:ARG:NH1	1:B:658:ARG:HG3	2.29	0.45
1:B:872:THR:HG23	1:B:874:SER:N	2.31	0.45
1:A:739:ARG:CB	1:A:953:HIS:CG	3.00	0.45
1:A:492:GLN:HG2	1:A:493:LYS:HE2	1.98	0.45
1:A:777:VAL:HG12	1:A:778:LYS:N	2.31	0.45
1:A:815:GLU:CD	1:A:832:HIS:NE2	2.69	0.45
3:D:6:DC:O2	4:E:27:DG:N1	2.48	0.45
1:A:615:ILE:HG22	1:A:619:MET:CE	2.46	0.45
1:B:462:LEU:HD23	1:B:528:LYS:HG2	1.99	0.45
1:B:813:SER:O	1:B:817:LEU:HG	2.16	0.45
4:E:18:DC:H2"	4:E:19:DG:C8	2.52	0.45
1:A:412:ALA:HA	1:A:415:GLN:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:MET:CE	1:A:533:GLN:HB3	2.47	0.45
1:A:975:GLU:HA	1:A:975:GLU:OE1	2.16	0.45
1:A:745:SER:HB2	1:A:985:HIS:CG	2.51	0.45
1:A:714:ASN:O	1:A:719:LEU:N	2.45	0.44
1:A:393:MET:HE1	1:A:393:MET:HA	1.99	0.44
1:B:552:PHE:CE2	1:B:575:LEU:N	2.83	0.44
1:B:386:VAL:HG12	1:B:393:MET:CE	2.47	0.44
4:E:22:DC:H2''	4:E:23:DG:OP2	2.17	0.44
1:B:619:MET:HE2	1:B:619:MET:HB2	1.80	0.44
1:B:764:HIS:CE1	1:B:765:LEU:HG	2.52	0.44
1:B:777:VAL:HG12	1:B:778:LYS:N	2.32	0.44
1:A:638:TRP:NE1	1:A:642:LYS:HE2	2.32	0.44
1:A:950:ASP:OD2	1:A:953:HIS:CG	2.67	0.44
1:B:980:ASN:OD1	1:A:459:GLU:HG2	2.18	0.44
1:B:714:ASN:ND2	1:B:714:ASN:N	2.63	0.44
1:B:644:HIS:CE1	1:B:646:SER:H	2.36	0.44
1:A:387:LEU:HD13	1:A:401:LYS:NZ	2.33	0.44
1:A:786:LEU:N	1:A:786:LEU:CD1	2.81	0.44
1:B:436:TYR:CB	1:B:439:ILE:HD12	2.48	0.44
1:A:431:MET:CE	1:A:535:VAL:HG13	2.48	0.43
1:B:410:LEU:HD12	1:B:415:GLN:CA	2.47	0.43
1:B:651:GLU:HG2	1:B:698:ILE:HG21	1.99	0.43
1:A:428:TRP:C	1:A:429:ILE:HG13	2.38	0.43
1:A:893:ALA:CB	1:A:901:TRP:HZ3	2.31	0.43
1:B:579:LEU:HD13	1:B:582:MET:HE3	1.99	0.43
1:B:593:THR:HG21	1:B:653:LEU:HD22	1.99	0.43
1:B:474:ALA:HB3	1:B:475:PRO:CD	2.48	0.43
1:B:421:LEU:HD23	1:B:424:ARG:HD2	2.00	0.43
1:A:457:GLN:HE21	1:A:457:GLN:HB3	1.61	0.43
1:A:493:LYS:CB	1:A:493:LYS:HZ3	2.32	0.43
1:A:706:ARG:NH1	1:A:706:ARG:HB3	2.34	0.43
1:A:753:LEU:O	1:A:759:CYS:HB2	2.19	0.43
1:B:428:TRP:C	1:B:429:ILE:HG13	2.38	0.43
1:B:411:SER:OG	1:B:449:GLU:CD	2.56	0.43
1:B:612:LEU:HD13	1:B:669:ILE:CG1	2.49	0.43
1:B:631:ALA:CB	1:B:673:PHE:CD1	2.99	0.43
1:B:761:LYS:HG2	1:B:761:LYS:H	1.58	0.43
1:B:906:TRP:O	1:B:910:GLU:HB2	2.18	0.43
3:D:1:DC:H1'	3:D:2:DG:H5'	2.01	0.43
1:B:717:GLN:C	1:B:718:HIS:CG	2.90	0.43
1:B:717:GLN:O	1:B:718:HIS:CG	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:848:ASP:O	1:B:852:MET:HB3	2.19	0.43
1:B:433:LYS:HA	1:B:433:LYS:HD3	1.85	0.43
1:A:456:LEU:HD21	1:A:535:VAL:HB	2.01	0.43
1:A:742:HIS:O	1:A:745:SER:HB3	2.19	0.43
1:A:436:TYR:HB3	1:A:439:ILE:HD12	2.01	0.43
1:B:681:HIS:HD2	1:A:441:LEU:O	2.02	0.43
1:A:741:GLY:O	1:A:985:HIS:CB	2.66	0.43
1:B:959:PRO:HG2	1:B:973:LEU:HB3	2.01	0.43
2:C:29:DC:H2"	2:C:30:DA:OP2	2.19	0.43
1:B:578:ASN:HB3	1:B:582:MET:SD	2.59	0.42
1:B:715:LEU:HA	1:B:719:LEU:CB	2.39	0.42
1:A:716:HIS:ND1	1:A:753:LEU:CG	2.82	0.42
1:A:840:THR:CG2	1:A:922:PHE:CE2	3.00	0.42
1:A:395:LEU:HD13	1:A:596:PHE:HB2	2.01	0.42
1:A:719:LEU:CD1	1:A:721:ARG:NH1	2.71	0.42
1:A:906:TRP:O	1:A:910:GLU:HB2	2.20	0.42
1:B:595:ILE:HG12	1:B:657:LEU:HD22	2.01	0.42
1:B:833:GLY:CA	1:B:837:THR:OG1	2.53	0.42
1:A:433:LYS:HA	1:A:433:LYS:HD3	1.81	0.42
1:A:579:LEU:HD13	1:A:582:MET:HE2	2.00	0.42
1:A:894:PRO:HG2	1:A:897:SER:H	1.84	0.42
1:A:975:GLU:OE2	1:A:987:GLN:NE2	2.53	0.42
1:B:874:SER:HA	1:B:877:THR:OG1	2.19	0.42
1:B:937:GLY:O	1:B:941:SER:HB3	2.19	0.42
1:A:612:LEU:HD13	1:A:669:ILE:HG12	2.01	0.42
1:A:492:GLN:CG	1:A:493:LYS:HE2	2.50	0.42
1:B:659:CYS:HA	1:B:664:TRP:CG	2.53	0.42
1:A:457:GLN:OE1	1:A:536:ARG:NH2	2.41	0.42
1:A:841:LEU:HD11	1:A:931:LEU:HD23	2.00	0.42
1:B:493:LYS:HA	1:B:493:LYS:HD3	1.71	0.42
1:B:903:ALA:CA	1:B:925:LEU:HD11	2.48	0.42
1:A:604:ARG:HD2	1:A:641:LEU:HG	2.02	0.42
1:A:376:LEU:O	1:A:380:LEU:HG	2.20	0.42
1:B:979:PRO:HD3	1:B:1006:VAL:O	2.20	0.42
1:B:672:ARG:HG2	1:B:672:ARG:H	1.52	0.42
1:B:478:LYS:HE3	1:B:489:PRO:HB2	2.02	0.41
1:B:895:GLU:CG	1:B:899:ARG:HD2	2.50	0.41
1:A:655:LEU:HD22	1:A:701:PRO:HG3	2.01	0.41
1:A:815:GLU:HG2	1:A:815:GLU:H	1.65	0.41
1:A:902:VAL:HG21	1:A:932:VAL:HG11	2.03	0.41
1:A:979:PRO:O	1:A:980:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:LEU:CD1	1:B:415:GLN:CA	2.98	0.41
1:B:615:ILE:HD11	1:B:631:ALA:HA	2.01	0.41
1:A:761:LYS:HG2	1:A:761:LYS:H	1.52	0.41
1:A:434:LEU:HD11	1:A:535:VAL:HG21	2.02	0.41
1:A:814:VAL:CG2	1:A:815:GLU:N	2.83	0.41
1:A:946:HIS:CB	1:A:954:CYS:SG	3.08	0.41
1:B:393:MET:HB3	1:B:401:LYS:CE	2.50	0.41
1:B:880:ARG:N	1:B:881:PRO:HD2	2.36	0.41
1:A:739:ARG:CB	1:A:953:HIS:CD2	3.04	0.41
1:A:977:LYS:O	1:A:1005:HIS:HA	2.21	0.41
1:A:979:PRO:HD3	1:A:1006:VAL:O	2.20	0.41
1:B:558:MET:H	1:B:558:MET:HG2	1.70	0.41
3:D:10:DC:H2'	3:D:10:DC:H6	1.75	0.41
4:E:22:DC:H6	4:E:22:DC:H2'	1.64	0.41
1:A:554:LEU:HD12	1:A:595:ILE:HD13	2.02	0.41
1:B:411:SER:O	1:B:414:GLY:N	2.54	0.41
1:B:545:PHE:HA	1:B:548:ILE:HD12	2.01	0.41
3:D:8:DA:H2''	3:D:9:DG:OP2	2.21	0.41
1:A:387:LEU:HD13	1:A:401:LYS:HZ2	1.86	0.41
1:A:611:MET:HG2	1:A:634:ALA:HB2	2.03	0.41
1:A:715:LEU:N	1:A:715:LEU:HD23	2.36	0.41
1:A:782:ILE:HG13	1:A:1006:VAL:HA	2.03	0.41
1:A:829:GLN:CB	1:A:964:TRP:CE2	3.02	0.41
1:B:639[B]:ASN:C	1:B:639[B]:ASN:OD1	2.59	0.41
1:B:906:TRP:CD1	1:B:906:TRP:C	2.94	0.41
1:A:936:GLY:O	1:A:940:LEU:HD12	2.21	0.41
1:A:937:GLY:N	1:A:938:PRO:CD	2.83	0.41
1:B:474:ALA:O	1:B:475:PRO:C	2.58	0.41
1:B:536:ARG:HH22	1:B:539:LYS:HE3	1.86	0.41
1:B:536:ARG:NH2	1:B:539:LYS:HE3	2.35	0.41
1:B:869:ASP:O	1:B:875:PHE:HB2	2.21	0.41
1:A:558:MET:HB2	1:A:668:ARG:CZ	2.51	0.41
1:A:726:ILE:HD12	1:A:766:PHE:CE1	2.56	0.41
1:B:832:HIS:CE1	1:B:834:GLU:OE2	2.73	0.41
1:A:760:LYS:O	1:A:763:LYS:CD	2.68	0.41
1:A:833:GLY:HA3	1:A:921:ARG:HE	1.85	0.41
1:A:390:GLU:CG	4:E:32:DG:H5''	2.32	0.41
1:A:384:LYS:HB3	1:A:384:LYS:HE3	1.95	0.40
1:A:583:GLU:HG2	1:A:912:ARG:HD3	2.02	0.40
1:B:488:ASN:C	1:B:490:ASN:H	2.25	0.40
1:B:678:GLN:HB2	1:B:678:GLN:HE21	1.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:640:ARG:HG3	1:B:640:ARG:O	2.21	0.40
1:B:779:HIS:CG	1:A:522:VAL:HG13	2.56	0.40
1:A:833:GLY:HA2	1:A:921:ARG:NH2	2.36	0.40
1:B:716:HIS:HB2	1:B:725:THR:HG21	2.03	0.40
1:B:744:LEU:CB	1:B:989:ILE:HD11	2.48	0.40
2:C:22:DT:H1'	2:C:23:DG:C8	2.56	0.40
1:A:628:LYS:HE3	1:A:682:MET:SD	2.61	0.40
1:A:741:GLY:HA3	1:A:986:LYS:HG3	2.04	0.40
1:A:760:LYS:HA	1:A:763:LYS:HZ2	1.86	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	583/647 (90%)	563 (97%)	19 (3%)	1 (0%)	47	78
1	B	581/647 (90%)	559 (96%)	22 (4%)	0	100	100
All	All	1164/1294 (90%)	1122 (96%)	41 (4%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	786	LEU

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	516/562 (92%)	462 (90%)	54 (10%)	7	30
1	B	515/562 (92%)	444 (86%)	71 (14%)	3	21
All	All	1031/1124 (92%)	906 (88%)	125 (12%)	5	25

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	371	GLU
1	B	376	LEU
1	B	387	LEU
1	B	390	GLU
1	B	409	GLN
1	B	411	SER
1	B	413	THR
1	B	429	ILE
1	B	442	ASP
1	B	455	PHE
1	B	457	GLN
1	B	465	LEU
1	B	478	LYS
1	B	486	LEU
1	B	487	VAL
1	B	490	ASN
1	B	495	GLN
1	B	501	LEU
1	B	526	ARG
1	B	539	LYS
1	B	549	LEU
1	B	579	LEU
1	B	591	ARG
1	B	595	ILE
1	B	628	LYS
1	B	640	ARG
1	B	641	LEU
1	B	642	LYS
1	B	648	ARG
1	B	652	ASP
1	B	672	ARG
1	B	678	GLN
1	B	688	ARG
1	B	706	ARG

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Mol	Chain	Res	Type
1	B	714	ASN
1	B	715	LEU
1	B	718	HIS
1	B	722	LEU
1	B	728	CYS
1	B	744	LEU
1	B	749	ARG
1	B	758	SER
1	B	760	LYS
1	B	761	LYS
1	B	768	GLN
1	B	774	VAL
1	B	816	GLU
1	B	834	GLU
1	B	836	SER
1	B	839	SER
1	B	848	ASP
1	B	866	PHE
1	B	873	ASP
1	B	874	SER
1	B	891	HIS
1	B	912	ARG
1	B	913	VAL
1	B	933	SER
1	B	941	SER
1	B	952	ARG
1	B	954	CYS
1	B	955	ARG
1	B	962	VAL
1	B	966	SER
1	B	981	ASP
1	B	982	ARG
1	B	985	HIS
1	B	990	TRP
1	B	1004	CYS
1	B	1006	VAL
1	B	1007	VAL
1	A	376	LEU
1	A	391	ASP
1	A	399	GLN
1	A	401	LYS
1	A	432	THR

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Mol	Chain	Res	Type
1	A	456	LEU
1	A	457	GLN
1	A	461	GLU
1	A	465	LEU
1	A	476	GLU
1	A	486	LEU
1	A	490	ASN
1	A	493	LYS
1	A	501	LEU
1	A	502	LYS
1	A	526	ARG
1	A	530	LEU
1	A	556	ASP
1	A	559	GLU
1	A	578	ASN
1	A	587	TYR
1	A	589	ILE
1	A	594	HIS
1	A	603	ILE
1	A	625	GLU
1	A	640	ARG
1	A	641	LEU
1	A	643	ASN
1	A	648	ARG
1	A	678	GLN
1	A	679	ARG
1	A	698	ILE
1	A	718	HIS
1	A	728	CYS
1	A	740	THR
1	A	748	GLN
1	A	754	ARG
1	A	758	SER
1	A	761	LYS
1	A	772	MET
1	A	776	ASP
1	A	785	ARG
1	A	786	LEU
1	A	787	CYS
1	A	811	LEU
1	A	872	THR
1	A	890	ILE

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Mol	Chain	Res	Type
1	A	916	LEU
1	A	918	SER
1	A	954	CYS
1	A	970	HIS
1	A	982	ARG
1	A	990	TRP
1	A	1000	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	678	GLN
1	B	718	HIS
1	B	907	HIS
1	B	953	HIS
1	B	1005	HIS
1	A	452	ASN
1	A	678	GLN
1	A	714	ASN
1	A	953	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](#)

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	590/647 (91%)	0.14	47 (7%) 12 10	143, 219, 293, 355	0
1	B	588/647 (90%)	-0.01	25 (4%) 35 29	145, 210, 276, 432	0
2	C	10/10 (100%)	-0.06	0 100 100	232, 246, 258, 274	0
3	D	10/10 (100%)	-0.76	0 100 100	201, 212, 236, 238	0
4	E	17/17 (100%)	-0.01	3 (17%) 1 1	190, 222, 263, 284	0
All	All	1215/1331 (91%)	0.06	75 (6%) 20 16	143, 215, 287, 432	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	758	SER	6.7
1	A	558	MET	6.7
1	A	1002	GLU	5.6
1	A	999	ALA	5.2
1	A	740	THR	4.8
1	A	772	MET	4.7
1	A	771	GLU	4.5
1	A	757	PRO	4.5
1	B	455	PHE	4.4
1	A	831	ILE	4.4
1	B	759	CYS	4.3
1	A	557	SER	4.1
1	B	638	TRP	4.0
1	A	770	PRO	3.9
1	B	868	LEU	3.9
1	A	643	ASN	3.9
1	A	455	PHE	3.8
1	B	408	TYR	3.8
1	B	757	PRO	3.8
1	A	596	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
4	E	16	DG	3.7
1	A	409	GLN	3.6
1	A	726	ILE	3.6
1	A	972	LYS	3.6
1	A	708	TRP	3.6
1	A	868	LEU	3.3
1	B	552	PHE	3.3
1	A	759	CYS	3.3
1	B	407	PHE	3.3
4	E	17	DG	3.3
1	A	733	LEU	3.0
1	B	831	ILE	3.0
1	A	729	ILE	2.9
1	A	559	GLU	2.9
1	B	656	PHE	2.9
1	A	669	ILE	2.9
1	B	709	ASP	2.8
1	B	557	SER	2.8
1	B	758	SER	2.8
1	B	857	ASP	2.8
1	A	589	ILE	2.8
1	B	439	ILE	2.7
1	A	1000	GLU	2.7
1	A	552	PHE	2.6
1	B	415	GLN	2.5
1	A	1001	VAL	2.5
1	A	753	LEU	2.5
1	B	771	GLU	2.5
1	A	657	LEU	2.5
4	E	18	DC	2.5
1	A	709	ASP	2.4
1	A	408	TYR	2.4
1	A	410	LEU	2.4
1	B	981	ASP	2.4
1	B	844	LEU	2.4
1	B	766	PHE	2.4
1	A	621	ASN	2.4
1	A	723	GLU	2.4
1	A	700	CYS	2.3
1	A	556	ASP	2.3
1	A	644	HIS	2.3
1	B	417	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1002	GLU	2.2
1	A	668	ARG	2.2
1	B	769	LEU	2.1
1	A	707	TRP	2.1
1	A	471	LEU	2.1
1	B	416	LYS	2.1
1	A	832	HIS	2.0
1	A	973	LEU	2.0
1	A	971	PHE	2.0
1	B	863	CYS	2.0
1	A	418	TYR	2.0
1	A	774	VAL	2.0
1	A	743	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.