



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:18 PM GMT

PDB ID : 4REA
Title : A Nuclease DNA complex
Authors : Zhao, Q.; Xue, X.; Longerich, S.; Sung, P.; Xiong, Y.
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

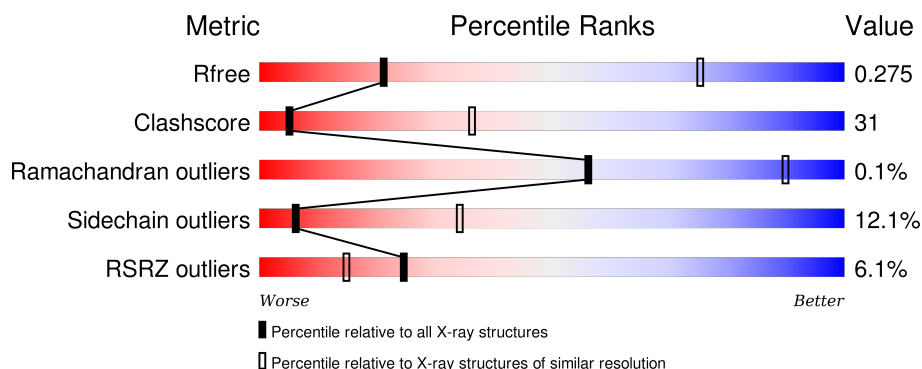
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.81 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}	91344	1324 (4.14-3.50)
Clashscore	102246	1028 (4.12-3.52)
Ramachandran outliers	100387	1404 (4.14-3.50)
Sidechain outliers	100360	1399 (4.14-3.50)
RSRZ outliers	91569	1332 (4.14-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	647	 7% 52% 35% 9%
1	B	647	 4% 51% 34% 6% 9%
2	C	10	 20% 80%
3	D	10	 10% 90%
4	E	17	 18% 24% 76%

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			

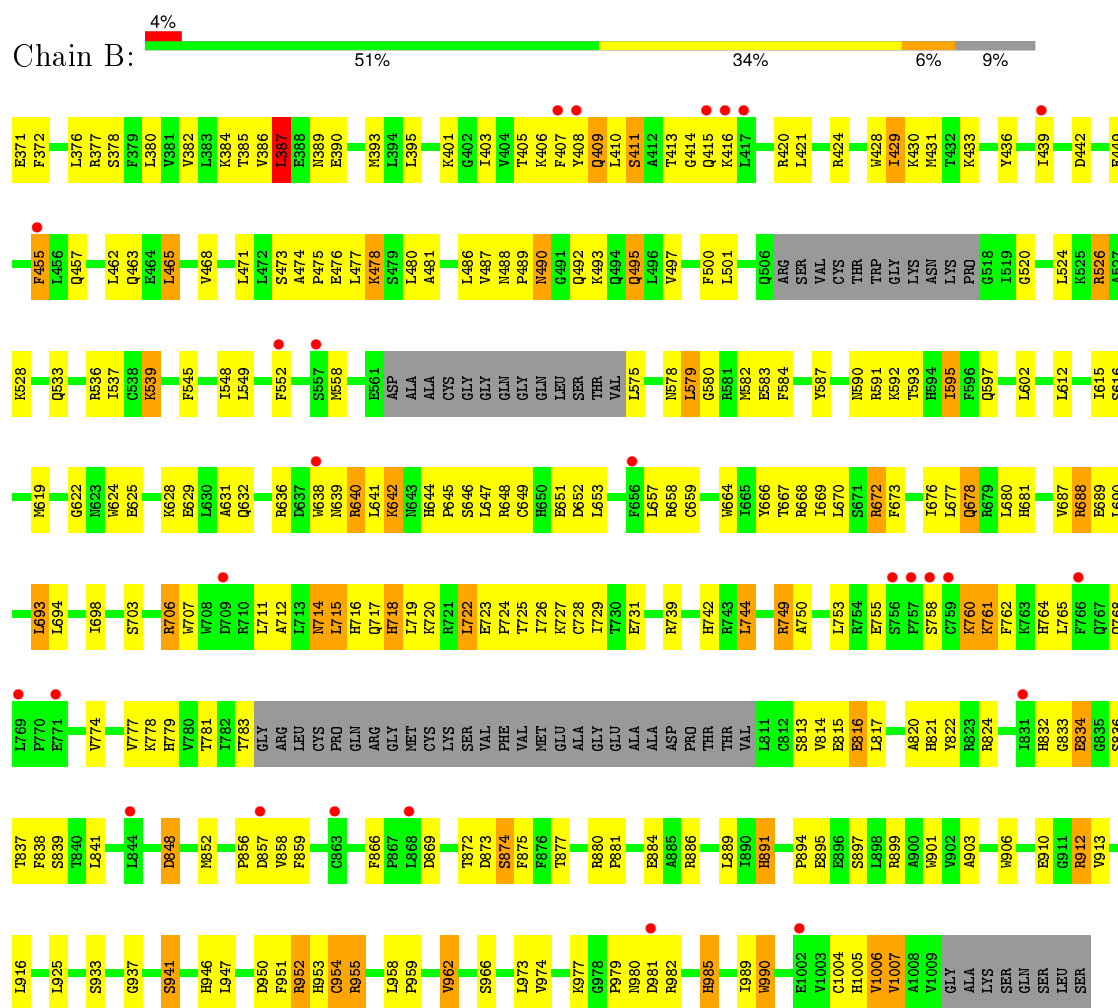
- Molecule 4 is a DNA chain called DNA (5'-D(P*GP*GP*CP*GP*AP*GP*CP*GP*CP*TP*CP*GP*CP*CP*AP*CP*G)-3').

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

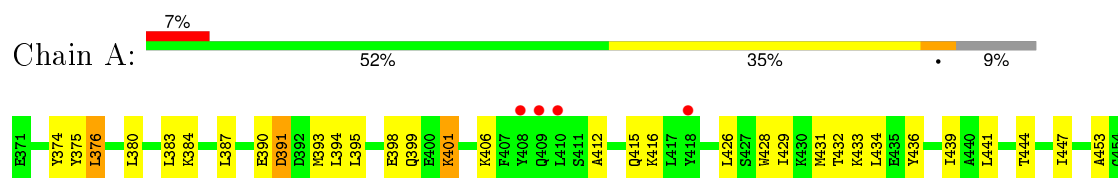
3 Residue-property plots

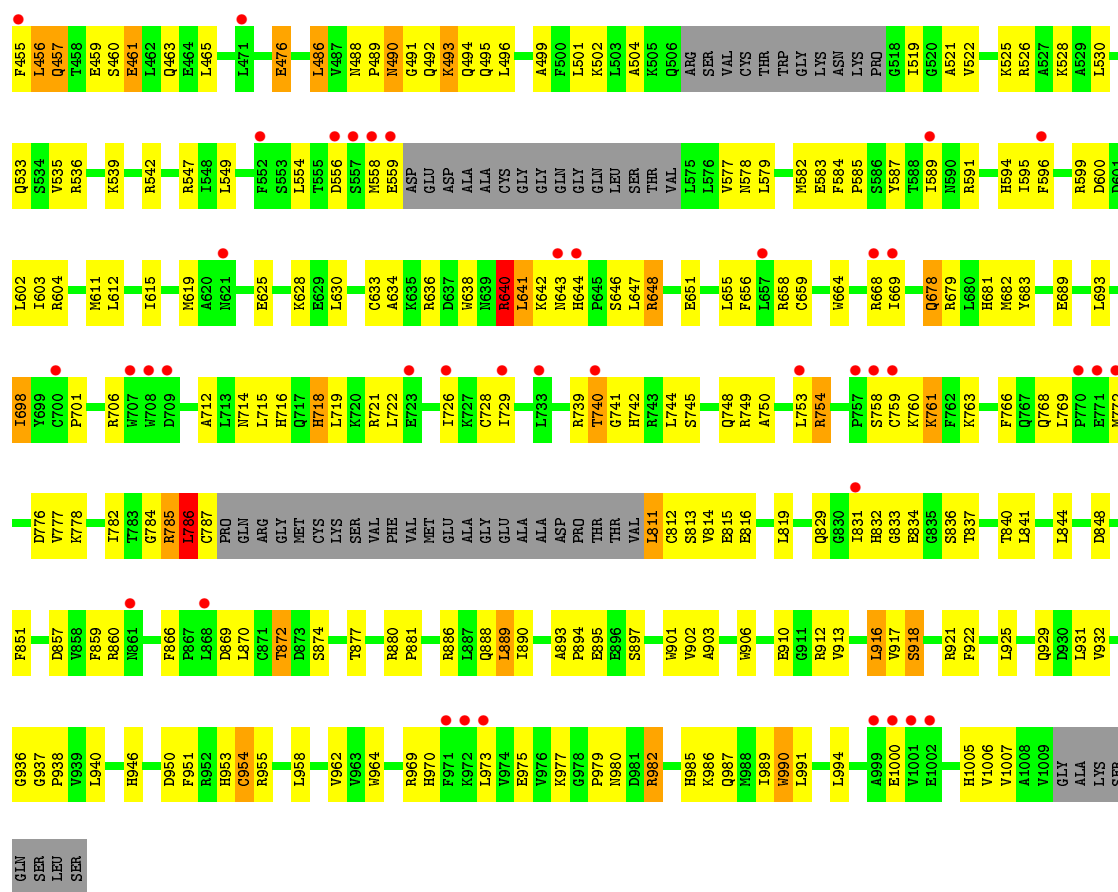
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: Fanconi-associated nuclease 1



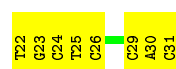
- Molecule 1: Fanconi-associated nuclease 1





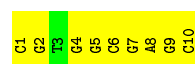
- Molecule 2: DNA (5'-D(*TP*GP*CP*TP*CP*GP*CP*CP*AP*C)-3')

Chain C: 20% 80%



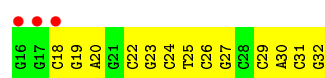
- Molecule 3: DNA (5'-D(P*CP*GP*TP*GP*GP*CP*GP*AP*GP*C)-3')

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 0.246 , 0.275	Depositor DCC
R_{free} test set	613 reflections (4.86%)	DCC
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
Estimated twinning fraction	0.490 for H, K, L 0.510 for K, H, -L 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
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
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.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.55	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
1:A:390:GLU:HG3	4:E:32:DG:H5"	1.42	1.00
3:D:7:DG:N2	4:E:26:DC:N3	2.06	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:950:ASP:OD1	1:A:953:HIS:CD2	2.20	0.94
1:A:461:GLU:OE1	1:A:461:GLU:O	1.85	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:HE2	1:A:493:LYS:H	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:813:SER:HG	1:A:816:GLU:CG	1.88	0.83
1:A:493:LYS:CE	1:A:493:LYS:H	1.92	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:B:822:TYR:CE2	1:B:974:VAL:HG21	2.15	0.82
1:A:579:LEU:HD12	1:A:584:PHE:HZ	1.44	0.82
1:B:727:LYS:O	1:B:731:GLU:HG3	1.79	0.82
1:A:832:HIS:O	1:A:832:HIS:ND1	2.11	0.81
1:A:644:HIS:CE1	1:A:646:SER:H	1.98	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:813:SER:HG	1:B:816:GLU:H	1.29	0.78
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: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:B:409:GLN:NE2	1:B:409:GLN:H	1.84	0.75
1:A:815:GLU:CG	1:A:832:HIS:CD2	2.68	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:B:954:CYS:HG	1:B:990:TRP:HZ2	1.36	0.72
1:A:644:HIS:HE1	1:A:646:SER:HB3	1.54	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:B:410:LEU:HD23	1:B:449:GLU:CD	2.09	0.71
1:A:872:THR:HG23	1:A:874:SER:H	1.54	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:B:834:GLU:N	1:B:834:GLU:OE1	2.25	0.69
1:A:426:LEU:HD13	1:A:542:ARG:HD2	1.73	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:B:410:LEU:CD1	1:B:414:GLY:CA	2.67	0.68
1:B:410:LEU:HD22	1:B:449:GLU:OE2	1.93	0.68
1:B:410:LEU:HD13	1:B:411:SER:O	1.94	0.68
1:A:493:LYS:H	1:A:493:LYS:NZ	1.92	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:B:410:LEU:HD11	1:B:414:GLY:O	1.91	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: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: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:A:729:ILE:HG21	1:A:750:ALA:HB2	1.77	0.66
1:B:815:GLU:HB3	1:B:832:HIS:HD2	1.58	0.66
1:B:668:ARG:O	1:B:672:ARG:HG2	1.96	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:HG3	1:B:658:ARG:HH11	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:894:PRO:HG2	1:A:897:SER:CB	2.27	0.65
1:A:644:HIS:CE1	1:A:646:SER:HG	2.13	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:B:717:GLN:HB3	1:B:718:HIS:CD2	2.31	0.64
1:A:829:GLN:HB2	1:A:964:TRP:CE2	2.32	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:A:401:LYS:HE2	3:D:5:DG:OP1	1.98	0.63
1:B:477:LEU:HD21	1:B:497:VAL:HG23	1.80	0.63
3:D:1:DC:C4	4:E:32:DG:O6	2.50	0.63
3:D:8:DA:N1	4:E:25:DT:O4	2.32	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:821:HIS:HA	1:B:824:ARG:HE	1.64	0.62
1:B:424:ARG:HG2	2:C:30:DA:H5"	1.81	0.62
1:A:493:LYS:HZ3	1:A:493:LYS:H	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:894:PRO:CD	1:A:897:SER:OG	2.49	0.60
1:A:547:ARG:HB3	1:A:602:LEU:HD21	1.82	0.60
1:A:584:PHE:O	1:A:912:ARG:HD2	2.00	0.60
1:B:1005:HIS:CD2	1:A:525:LYS:HG2	2.37	0.60
1:A:585:PRO:HD3	1:A:913:VAL:O	2.02	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
3:D:1:DC:O2	4:E:32:DG:N1	2.30	0.59
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
1:B:552:PHE:HE2	1:B:575:LEU:N	2.00	0.59
1:A:659:CYS:HA	1:A:664:TRP:CG	2.37	0.59
1:A:644:HIS:CE1	1:A:646:SER:N	2.70	0.59
1:A:547:ARG:HD2	1:A:602:LEU:HG	1.84	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:B:410:LEU:HD21	1:B:414:GLY:HA3	1.83	0.59
1:B:436:TYR:HE1	2:C:31:DC:OP1	1.86	0.59
1:B:680:LEU:HD22	1:A:441:LEU:HD13	1.85	0.59
1:A:611:MET:SD	1:A:634:ALA:HB2	2.43	0.59
1:B:977:LYS:HB2	1:B:1005:HIS:CD2	2.37	0.59
1:A:786:LEU:CD2	1:A:812:CYS:SG	2.90	0.59
1:B:377:ARG:HG2	1:B:580:GLY:HA3	1.85	0.59
1:A:786:LEU:HB2	1:A:811:LEU:HA	1.82	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

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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:456:LEU:HD23	1:A:536:ARG:O	2.03	0.57
1:A:374:TYR:CE2	1:A:577:VAL:HG13	2.39	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:813:SER:OG	1:B:816:GLU:CG	2.52	0.56
1:B:644:HIS:HE1	1:B:646:SER:HB3	1.70	0.56
1:B:952:ARG:HB2	1:B:952:ARG:CZ	2.35	0.56
1:A:492:GLN:O	1:A:495:GLN:HG2	2.04	0.56
1:B:424:ARG:HG2	2:C:30:DA:C5'	2.35	0.56
1:A:745:SER:HB2	1:A:985:HIS:CD2	2.40	0.56
1:A:490:ASN:OD1	1:A:490:ASN:N	2.39	0.56
1:B:783:THR:HA	1:B:1007:VAL:HG22	1.86	0.56
1:B:952:ARG:NH1	1:B:952:ARG:HB3	2.20	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: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:HG2	1:B:755:GLU:O	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
4:E:29:DC:H2''	4:E:30:DA:C8	2.41	0.56
1:B:583:GLU:CB	1:B:912:ARG:HE	2.17	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:840:THR:CG2	1:A:922:PHE:HE2	2.20	0.56
1:B:616:SER:HA	1:B:619:MET:CE	2.35	0.55
1:B:492:GLN:O	1:B:495:GLN:HG2	2.06	0.55
1:A:848:ASP:OD1	1:A:886:ARG:NH2	2.36	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:B:815:GLU:CB	1:B:832:HIS:CD2	2.88	0.55
1:B:712:ALA:HA	1:B:715:LEU:HD13	1.88	0.55
1:B:903:ALA:HA	1:B:925:LEU:CD1	2.36	0.55
1:A:642:LYS:O	1:A:647:LEU:HD12	2.06	0.55
1:B:411:SER:HG	1:B:449:GLU:CD	2.09	0.55
1:A:714:ASN:HA	1:A:718:HIS:HB2	1.89	0.55
1:A:579:LEU:HD13	1:A:582:MET:CE	2.37	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:B:838:PHE:HA	1:B:841:LEU:HD12	1.89	0.54
1:A:636:ARG:HB2	1:A:636:ARG:NH1	2.22	0.54
1:B:430:LYS:NZ	1:B:476:GLU:OE1	2.39	0.54
1:A:376:LEU:HD22	1:A:380:LEU:CD1	2.36	0.54
1:A:579:LEU:CD1	1:A:584:PHE:CE2	2.90	0.54
1:A:656:PHE:HB2	1:A:869:ASP:HA	1.89	0.54
1:A:615:ILE:HG22	1:A:619:MET:HE2	1.90	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: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:A:391:ASP:HA	1:A:394:LEU:HD12	1.90	0.54
1:B:880:ARG:O	1:B:884:GLU:HG2	2.08	0.54
1:B:430:LYS:HG3	1:B:471:LEU:HD11	1.91	0.53
1:A:844:LEU:HD13	1:A:902:VAL:HG13	1.88	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:947:LEU:HD23	1:B:954:CYS:HB3	1.89	0.53
1:B:481:ALA:CA	1:B:500:PHE:HZ	2.19	0.53
1:B:410:LEU:HD22	1:B:449:GLU:CD	2.27	0.53
1:B:706:ARG:CB	1:B:706:ARG:HH11	2.22	0.53
1:A:640:ARG:O	1:A:640:ARG:CZ	2.57	0.53
1:B:465:LEU:HD21	1:B:520:GLY:HA2	1.89	0.53
1:A:406:LYS:HG3	1:A:455:PHE:HE2	1.74	0.53
1:B:858:VAL:HG23	1:B:859:PHE:CD2	2.44	0.53
1:B:722:LEU:O	1:B:726:ILE:HG12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:582:MET:HG3	1:B:584:PHE:CE1	2.44	0.53
1:B:431:MET:HE3	1:B:533:GLN:HB3	1.90	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:648:ARG:HB3	1:A:648:ARG:CZ	2.38	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:A:416:LYS:HD2	1:A:439:ILE:HG12	1.90	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:754:ARG:HD3	1:A:766:PHE:CB	2.39	0.52
1:A:716:HIS:CE1	1:A:753:LEU:HD21	2.45	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:813:SER:HB3	1:B:816:GLU:CG	2.32	0.52
1:B:411:SER:OG	1:B:449:GLU:OE2	2.27	0.52
1:B:409:GLN:N	1:B:409:GLN:NE2	2.55	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:B:916:LEU:HD23	1:B:951:PHE:CZ	2.46	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:A:903:ALA:HB2	1:A:929:GLN:NE2	2.25	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:B:955:ARG:HG3	1:B:955:ARG:HH11	1.75	0.51
1:A:987:GLN:O	1:A:991:LEU:HG	2.10	0.51
1:B:436:TYR:CE1	2:C:31:DC:OP1	2.63	0.51
1:A:491:GLY:O	1:A:496:LEU:HG	2.10	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:HB3	1:B:706:ARG:HH11	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:814:VAL:HG23	1:A:815:GLU:N	2.26	0.50
1:A:754:ARG:O	1:A:754:ARG:CG	2.55	0.50
1:A:785:ARG:O	1:A:786:LEU:HB2	2.12	0.50
1:A:476:GLU:OE1	1:A:476:GLU:HA	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:B:815:GLU:HB3	1:B:832:HIS:CD2	2.43	0.49
1:A:834:GLU:OE1	1:A:834:GLU:N	2.45	0.49
1:A:401:LYS:NZ	3:D:5:DG:OP1	2.46	0.49
1:B:416:LYS:HB3	1:B:439:ILE:HG12	1.94	0.49
1:B:403:ILE:HA	1:B:406:LYS:HE2	1.93	0.49
1:B:587:TYR:CD1	1:B:859:PHE:HB3	2.47	0.49
1:B:463:GLN:HA	1:B:524:LEU:HD21	1.93	0.49
1:A:591:ARG:HE	1:A:860:ARG:HB3	1.77	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:B:703:SER:HB2	1:B:707:TRP:CE2	2.46	0.49
1:B:378:SER:OG	1:B:575:LEU:O	2.28	0.49
1:A:888:GLN:HA	1:A:888:GLN:OE1	2.12	0.49
1:B:886:ARG:HD3	1:B:889:LEU:HD23	1.95	0.49
1:A:744:LEU:HB2	1:A:989:ILE:HD11	1.94	0.49
1:A:951:PHE:CZ	1:A:955:ARG:HD2	2.48	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:B:717:GLN:C	1:B:718:HIS:CD2	2.85	0.48
1:A:428:TRP:O	1:A:429:ILE:HG13	2.14	0.48
3:D:8:DA:H2	4:E:25:DT:H3	1.54	0.48
1:B:760:LYS:HG3	1:B:761:LYS:N	2.28	0.48
1:A:387:LEU:HD11	1:A:401:LYS:HZ1	1.78	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
2:C:25:DT:H2''	2:C:26:DC:O5'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:HIS:HA	1:A:683:TYR:CZ	2.47	0.48
1:B:814:VAL:CG2	1:B:815:GLU:N	2.76	0.48
1:A:722:LEU:O	1:A:726:ILE:HG12	2.14	0.48
1:A:488:ASN:N	1:A:489:PRO:HD3	2.29	0.48
1:A:786:LEU:N	1:A:786:LEU:HD12	2.28	0.48
1:A:493:LYS:HZ3	1:A:493:LYS:HB3	1.76	0.48
1:A:741:GLY:O	1:A:985:HIS:HB2	2.12	0.48
1:A:633:CYS:HA	1:A:636:ARG:HH12	1.78	0.48
1:B:673:PHE:O	1:B:677:LEU:HG	2.12	0.48
1:A:982:ARG:N	1:A:982:ARG:HD3	2.29	0.48
1:A:894:PRO:HD2	1:A:897:SER:CB	2.44	0.48
1:B:952:ARG:CB	1:B:952:ARG:NH1	2.76	0.48
1:B:952:ARG:HH11	1:B:952:ARG:HB3	1.78	0.48
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:A:638:TRP:O	1:A:642:LYS:HG3	2.14	0.47
1:A:636:ARG:CB	1:A:636:ARG:HH11	2.27	0.47
1:B:592:LYS:HB2	1:B:857:ASP:OD2	2.13	0.47
1:B:424:ARG:NE	2:C:30:DA:H5"	2.29	0.47
1:A:857:ASP:OD1	1:A:860:ARG:NH1	2.47	0.47
1:B:410:LEU:HD12	1:B:415:GLN:HA	1.96	0.47
1:B:377:ARG:CG	1:B:580:GLY:HA3	2.44	0.47
1:B:622:GLY:HA2	1:B:624:TRP:NE1	2.28	0.47
1:B:951:PHE:CD1	1:B:951:PHE:C	2.87	0.47
1:B:421:LEU:HB2	1:B:537:ILE:HD11	1.97	0.47
1:B:462:LEU:HD11	1:B:468:VAL:HB	1.97	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:B:1005:HIS:CD2	1:A:525:LYS:CE	2.96	0.47
1:B:716:HIS:ND1	1:B:749:ARG:NH1	2.62	0.47
1:A:374:TYR:CG	1:A:375:TYR:N	2.82	0.47
1:B:980:ASN:H	1:A:528:LYS:NZ	2.13	0.47
1:A:768:GLN:NE2	1:A:769:LEU:HG	2.29	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: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:A:777:VAL:HG12	1:A:778:LYS:H	1.80	0.47
3:D:1:DC:C2	4:E:32:DG:N1	2.79	0.47
1:B:420:ARG:O	1:B:424:ARG:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:LEU:HD22	1:A:719:LEU:N	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:B:410:LEU:HD13	1:B:415:GLN:N	2.24	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:A:426:LEU:HD21	1:A:539:LYS:HD3	1.97	0.46
1:B:632:GLN:HB3	1:B:636:ARG:HH12	1.81	0.46
1:A:903:ALA:HA	1:A:925:LEU:HD11	1.97	0.45
1:A:444:THR:HA	1:A:447:ILE:HD12	1.98	0.45
1:B:407:PHE:O	1:B:410:LEU:HB3	2.17	0.45
1:A:493:LYS:HE2	1:A:493:LYS:N	2.21	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:B:411:SER:OG	1:B:449:GLU:OE1	2.34	0.45
1:A:958:LEU:HD23	1:A:990:TRP:HD1	1.81	0.45
1:B:658:ARG:HG3	1:B:658:ARG:NH1	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:815:GLU:CD	1:A:832:HIS:NE2	2.69	0.45
1:A:492:GLN:HG2	1:A:493:LYS:HE2	1.98	0.45
3:D:6:DC:O2	4:E:27:DG:N1	2.48	0.45
1:A:777:VAL:HG12	1:A:778:LYS:N	2.31	0.45
1:A:615:ILE:HG22	1:A:619:MET:CE	2.46	0.45
1:B:813:SER:O	1:B:817:LEU:HG	2.16	0.45
1:B:462:LEU:HD23	1:B:528:LYS:HG2	1.99	0.45
4:E:18:DC:H2"	4:E:19:DG:C8	2.52	0.45
1:A:431:MET:CE	1:A:533:GLN:HB3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:SER:HB2	1:A:985:HIS:CG	2.51	0.45
1:A:975:GLU:HA	1:A:975:GLU:OE1	2.16	0.45
1:A:412:ALA:HA	1:A:415:GLN:OE1	2.16	0.45
1:A:714:ASN:O	1:A:719:LEU:N	2.45	0.44
1:B:552:PHE:CE2	1:B:575:LEU:N	2.83	0.44
1:A:393:MET:HE1	1:A:393:MET:HA	1.99	0.44
4:E:22:DC:H2''	4:E:23:DG:OP2	2.17	0.44
1:B:386:VAL:HG12	1:B:393:MET:CE	2.47	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:714:ASN:ND2	1:B:714:ASN:N	2.63	0.44
1:B:980:ASN:OD1	1:A:459:GLU:HG2	2.18	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:B:410:LEU:HD12	1:B:415:GLN:CA	2.47	0.43
1:A:431:MET:CE	1:A:535:VAL:HG13	2.48	0.43
1:B:651:GLU:HG2	1:B:698:ILE:HG21	1.99	0.43
1:B:593:THR:HG21	1:B:653:LEU:HD22	1.99	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:A:428:TRP:C	1:A:429:ILE:HG13	2.38	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:B:411:SER:OG	1:B:449:GLU:CD	2.56	0.43
3:D:1:DC:H1'	3:D:2:DG:H5'	2.01	0.43
1:A:493:LYS:CB	1:A:493:LYS:HZ3	2.32	0.43
1:A:753:LEU:O	1:A:759:CYS:HB2	2.19	0.43
1:B:631:ALA:CB	1:B:673:PHE:CD1	2.99	0.43
1:A:457:GLN:HE21	1:A:457:GLN:HB3	1.61	0.43
1:B:761:LYS:H	1:B:761:LYS:HG2	1.58	0.43
1:A:706:ARG:NH1	1:A:706:ARG:HB3	2.34	0.43
1:B:428:TRP:C	1:B:429:ILE:HG13	2.38	0.43
1:B:612:LEU:HD13	1:B:669:ILE:CG1	2.49	0.43
1:B:906:TRP:O	1:B:910:GLU:HB2	2.18	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
2:C:29:DC:H2"	2:C:30:DA:OP2	2.19	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:A:436:TYR:HB3	1:A:439:ILE:HD12	2.01	0.43
1:B:959:PRO:HG2	1:B:973:LEU:HB3	2.01	0.43
1:B:715:LEU:HA	1:B:719:LEU:CB	2.39	0.42
1:B:578:ASN:HB3	1:B:582:MET:SD	2.59	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:B:833:GLY:CA	1:B:837:THR:OG1	2.53	0.42
1:A:719:LEU:CD1	1:A:721:ARG:NH1	2.71	0.42
1:A:395:LEU:HD13	1:A:596:PHE:HB2	2.01	0.42
1:B:595:ILE:HG12	1:B:657:LEU:HD22	2.01	0.42
1:A:906:TRP:O	1:A:910:GLU:HB2	2.20	0.42
1:A:579:LEU:HD13	1:A:582:MET:HE2	2.00	0.42
1:A:433:LYS:HA	1:A:433:LYS:HD3	1.81	0.42
1:A:894:PRO:HG2	1:A:897:SER:H	1.84	0.42
1:B:874:SER:HA	1:B:877:THR:OG1	2.19	0.42
1:A:975:GLU:OE2	1:A:987:GLN:NE2	2.53	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: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: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: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:672:ARG:HG2	1:B:672:ARG:H	1.52	0.42
1:B:979:PRO:HD3	1:B:1006:VAL:O	2.20	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:B:410:LEU:CD1	1:B:415:GLN:CA	2.98	0.41
1:A:815:GLU:HG2	1:A:815:GLU:H	1.65	0.41
1:B:615:ILE:HD11	1:B:631:ALA:HA	2.01	0.41
1:A:655:LEU:HD22	1:A:701:PRO:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:761:LYS:HG2	1:A:761:LYS:H	1.52	0.41
1:A:946:HIS:CB	1:A:954:CYS:SG	3.08	0.41
1:A:814:VAL:CG2	1:A:815:GLU:N	2.83	0.41
1:B:393:MET:HB3	1:B:401:LYS:CE	2.50	0.41
1:A:434:LEU:HD11	1:A:535:VAL:HG21	2.02	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
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: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
1:A:977:LYS:O	1:A:1005:HIS:HA	2.21	0.41
1:B:411:SER:O	1:B:414:GLY:N	2.54	0.41
3:D:8:DA:H2''	3:D:9:DG:OP2	2.21	0.41
1:B:545:PHE:HA	1:B:548:ILE:HD12	2.01	0.41
1:A:554:LEU:HD12	1:A:595:ILE:HD13	2.02	0.41
1:A:387:LEU:HD13	1:A:401:LYS:HZ2	1.86	0.41
1:A:715:LEU:N	1:A:715:LEU:HD23	2.36	0.41
1:A:829:GLN:CB	1:A:964:TRP:CE2	3.02	0.41
1:A:611:MET:HG2	1:A:634:ALA:HB2	2.03	0.41
1:B:906:TRP:CD1	1:B:906:TRP:C	2.94	0.41
1:A:782:ILE:HG13	1:A:1006:VAL:HA	2.03	0.41
1:B:639[B]:ASN:C	1:B:639[B]:ASN:OD1	2.59	0.41
1:B:832:HIS:CE1	1:B:834:GLU:OE2	2.73	0.41
1:B:474:ALA:O	1:B:475:PRO:C	2.58	0.41
1:A:726:ILE:HD12	1:A:766:PHE:CE1	2.56	0.41
1:B:869:ASP:O	1:B:875:PHE:HB2	2.21	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: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:A:558:MET:HB2	1:A:668:ARG:CZ	2.51	0.41
1:A:390:GLU:CG	4:E:32:DG:H5''	2.32	0.41
1:A:833:GLY:HA3	1:A:921:ARG:HE	1.85	0.41
1:A:760:LYS:O	1:A:763:LYS:CD	2.68	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:678:GLN:HB2	1:B:678:GLN:HE21	1.59	0.40
1:B:488:ASN:C	1:B:490:ASN:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:779:HIS:CG	1:A:522:VAL:HG13	2.56	0.40
1:B:640:ARG:HG3	1:B:640:ARG:O	2.21	0.40
1:A:833:GLY:HA2	1:A:921:ARG:NH2	2.36	0.40
1:B:744:LEU:CB	1:B:989:ILE:HD11	2.48	0.40
1:B:716:HIS:HB2	1:B:725:THR:HG21	2.03	0.40
2:C:22:DT:H1'	2:C:23:DG:C8	2.56	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
1:A:628:LYS:HE3	1:A:682:MET:SD	2.61	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%)	52	86
1	B	581/647 (90%)	559 (96%)	22 (4%)	0	100	100
All	All	1164/1294 (90%)	1122 (96%)	41 (4%)	1 (0%)	56	90

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%)	8	41
1	B	515/562 (92%)	444 (86%)	71 (14%)	4	30
All	All	1031/1124 (92%)	906 (88%)	125 (12%)	6	34

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 ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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%)	0.17	45 (7%) 17 10	143, 219, 293, 355	0
1	B	588/647 (90%)	0.02	26 (4%) 38 25	145, 210, 276, 432	0
2	C	10/10 (100%)	-0.04	0 100 100	232, 246, 258, 274	0
3	D	10/10 (100%)	-0.75	0 100 100	201, 212, 236, 238	0
4	E	17/17 (100%)	0.02	3 (17%) 2 2	190, 222, 263, 284	0
All	All	1215/1331 (91%)	0.08	74 (6%) 25 15	143, 215, 287, 432	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	758	SER	6.9
1	A	558	MET	6.7
1	A	1002	GLU	5.7
1	A	999	ALA	5.3
1	A	740	THR	4.8
1	A	772	MET	4.7
1	A	771	GLU	4.6
1	B	759	CYS	4.5
1	B	455	PHE	4.4
1	A	757	PRO	4.4
1	A	831	ILE	4.4
1	A	557	SER	4.2
1	B	638	TRP	4.1
1	A	643	ASN	3.9
1	A	770	PRO	3.9
1	B	868	LEU	3.9
4	E	16	DG	3.9
1	A	455	PHE	3.8
1	B	408	TYR	3.8
1	A	596	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	757	PRO	3.7
1	A	409	GLN	3.6
1	A	708	TRP	3.6
1	A	726	ILE	3.5
1	A	759	CYS	3.5
1	A	972	LYS	3.5
4	E	17	DG	3.5
1	A	868	LEU	3.3
1	B	552	PHE	3.3
1	B	407	PHE	3.3
1	A	733	LEU	3.0
1	A	559	GLU	3.0
1	B	656	PHE	2.9
1	B	831	ILE	2.9
1	B	557	SER	2.9
1	B	709	ASP	2.9
1	A	669	ILE	2.9
1	A	729	ILE	2.9
1	B	758	SER	2.9
1	B	857	ASP	2.9
1	A	1000	GLU	2.8
1	A	589	ILE	2.7
1	B	439	ILE	2.7
1	A	552	PHE	2.6
1	B	415	GLN	2.6
1	B	771	GLU	2.5
1	A	709	ASP	2.5
1	A	700	CYS	2.5
1	A	1001	VAL	2.5
4	E	18	DC	2.5
1	A	753	LEU	2.5
1	A	657	LEU	2.5
1	A	408	TYR	2.4
1	B	981	ASP	2.4
1	A	723	GLU	2.4
1	A	410	LEU	2.4
1	A	621	ASN	2.4
1	B	766	PHE	2.4
1	B	844	LEU	2.4
1	A	556	ASP	2.3
1	B	1002	GLU	2.3
1	B	417	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	644	HIS	2.2
1	A	707	TRP	2.2
1	B	863	CYS	2.2
1	A	668	ARG	2.2
1	B	769	LEU	2.1
1	A	471	LEU	2.1
1	A	971	PHE	2.0
1	A	973	LEU	2.0
1	B	416	LYS	2.0
1	A	418	TYR	2.0
1	A	861	ASN	2.0
1	B	756	SER	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.