Full wwPDB X-ray Structure Validation Report ⓘ

Feb 11, 2024 – 08:57 AM EST

PDB ID	:	3C3L
Title	:	X-ray crystal structure of the N4 mini-vRNAP P2 promoter complex
Authors	:	Gleghorn, M.L.; Murakami, K.S.
Deposited on	:	2008-01-28
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

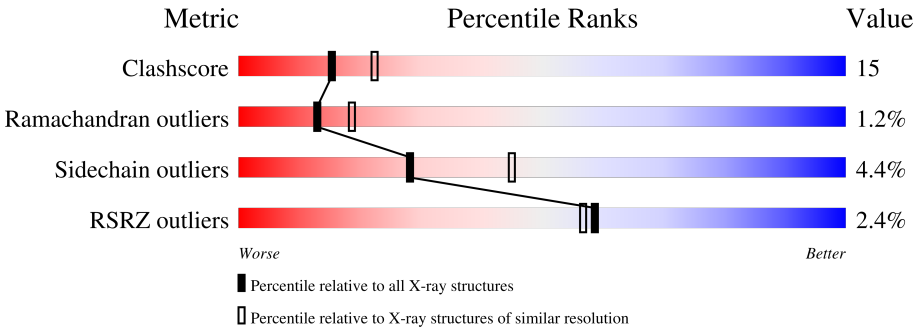
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	C	33	3% 27% 30% 42%
1	D	33	39% 18% 42%
2	A	1117	2% 69% 25%
2	B	1117	2% 70% 25%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17839 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 P2 Promoter DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	19	Total	C	N	O	P	0	0	0
			390	186	78	108	18			
1	D	19	Total	C	N	O	P	0	0	0
			390	186	78	108	18			

- Molecule 2 is a protein called Virion RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1089	Total	C	N	O	S	0	0	0
			8401	5274	1427	1659	41			
2	B	1085	Total	C	N	O	S	0	0	0
			8367	5254	1419	1653	41			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q859P9
A	-10	GLY	-	expression tag	UNP Q859P9
A	-9	GLY	-	expression tag	UNP Q859P9
A	-8	SER	-	expression tag	UNP Q859P9
A	-7	HIS	-	expression tag	UNP Q859P9
A	-6	HIS	-	expression tag	UNP Q859P9
A	-5	HIS	-	expression tag	UNP Q859P9
A	-4	HIS	-	expression tag	UNP Q859P9
A	-3	HIS	-	expression tag	UNP Q859P9
A	-2	HIS	-	expression tag	UNP Q859P9
A	-1	ARG	-	expression tag	UNP Q859P9
A	0	SER	-	expression tag	UNP Q859P9
B	-11	MET	-	expression tag	UNP Q859P9
B	-10	GLY	-	expression tag	UNP Q859P9
B	-9	GLY	-	expression tag	UNP Q859P9
B	-8	SER	-	expression tag	UNP Q859P9
B	-7	HIS	-	expression tag	UNP Q859P9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP Q859P9
B	-5	HIS	-	expression tag	UNP Q859P9
B	-4	HIS	-	expression tag	UNP Q859P9
B	-3	HIS	-	expression tag	UNP Q859P9
B	-2	HIS	-	expression tag	UNP Q859P9
B	-1	ARG	-	expression tag	UNP Q859P9
B	0	SER	-	expression tag	UNP Q859P9

- Molecule 3 is water.

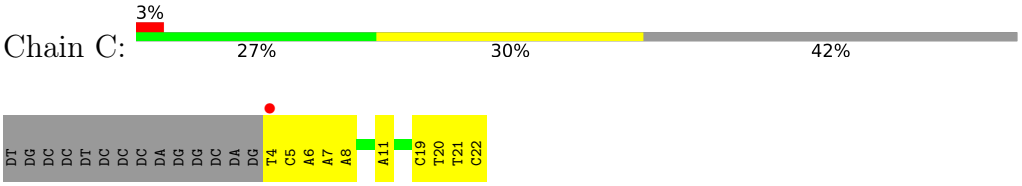
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	5	Total O 5 5	0	0
3	D	13	Total O 13 13	0	0
3	A	135	Total O 135 135	0	0
3	B	138	Total O 138 138	0	0

3 Residue-property plots (i)

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

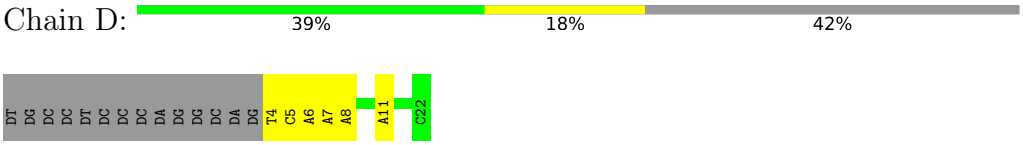
• Molecule 1: P2 Promoter DNA

Chain C:



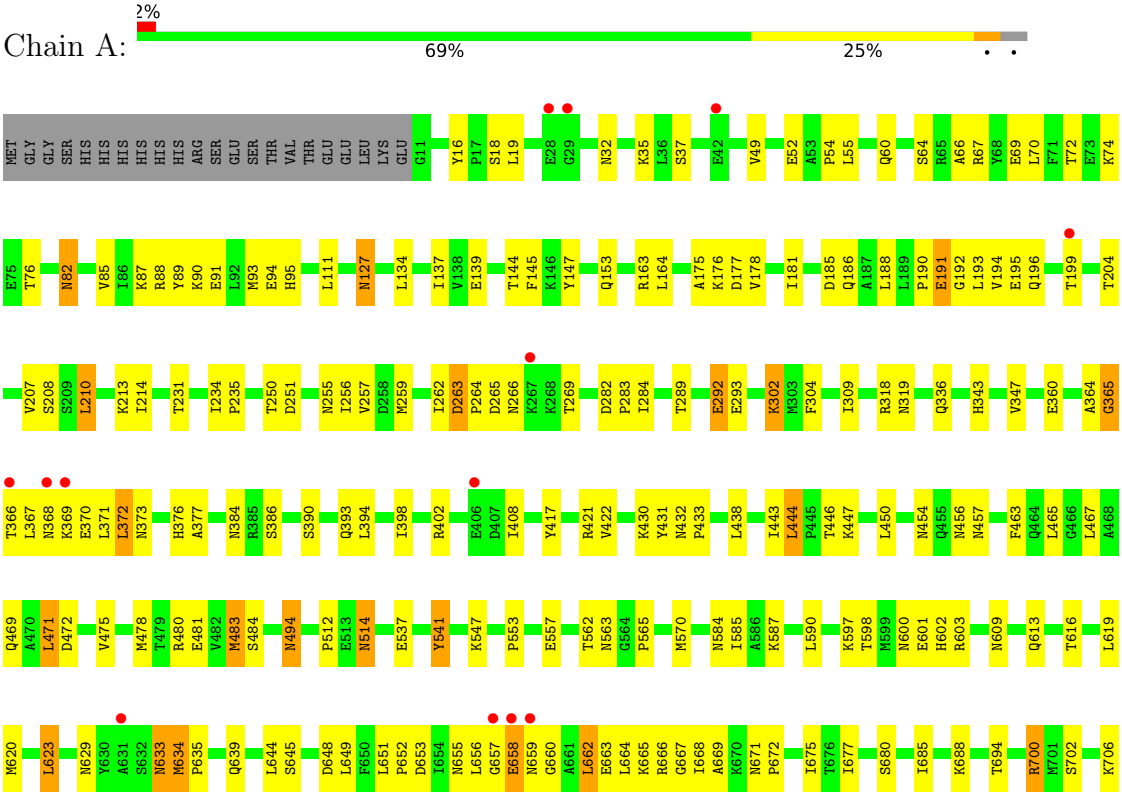
• Molecule 1: P2 Promoter DNA

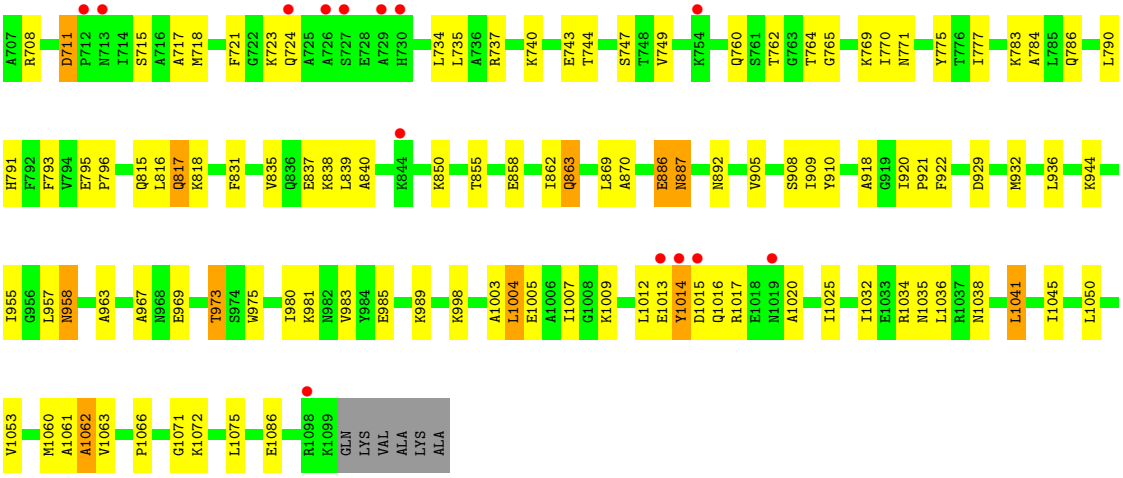
Chain D:



• Molecule 2: Virion RNA polymerase

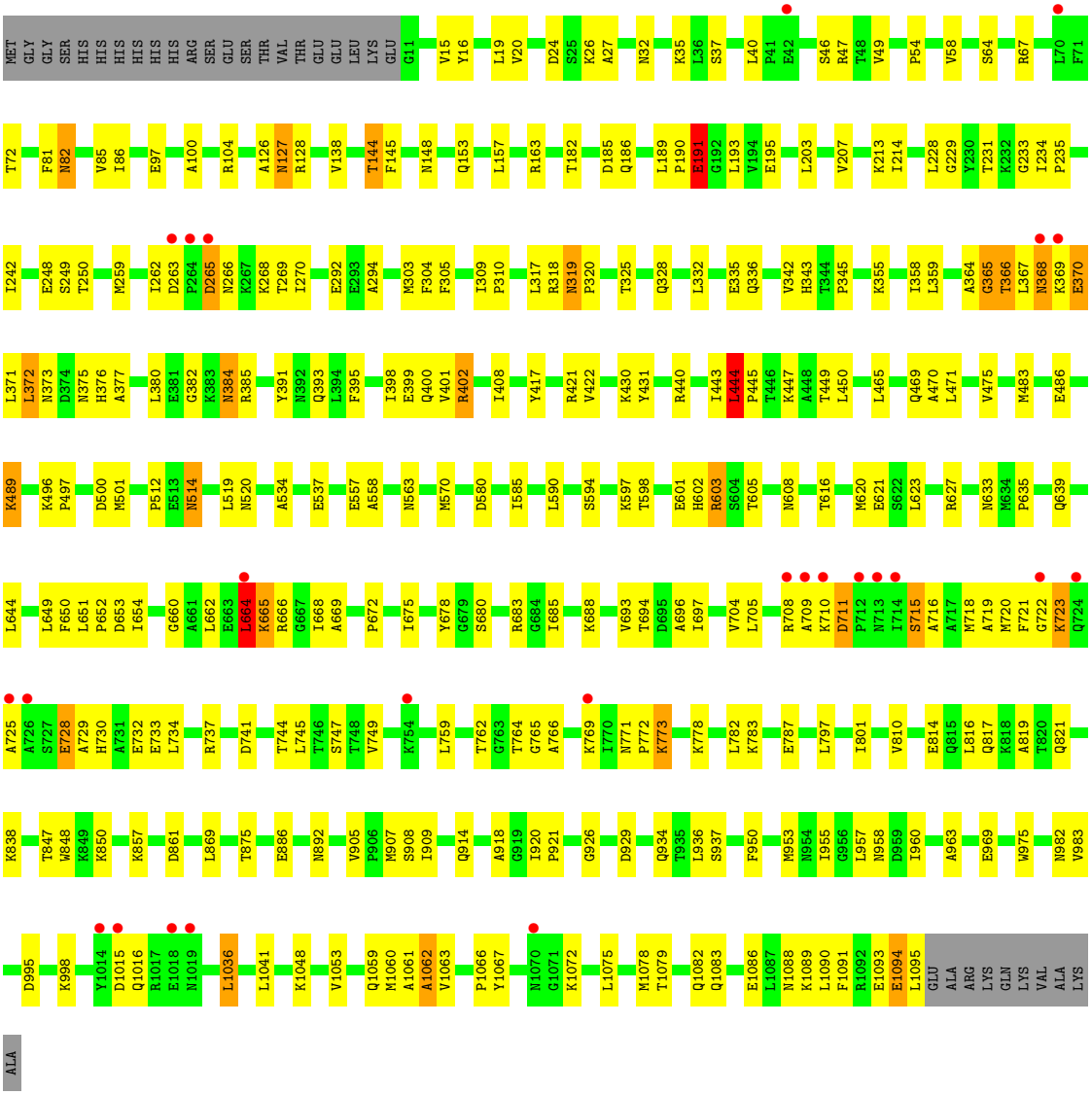
Chain A:





• Molecule 2: Virion RNA polymerase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.34Å 111.20Å 276.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 30.02 – 2.41	Depositor EDS
% Data completeness (in resolution range)	90.3 (30.00-2.40) 91.1 (30.02-2.41)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.59 (at 2.42Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.246 0.232 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	23.9	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 34.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	17839	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	C	0.35	0/439	0.69	0/676
1	D	0.34	0/439	0.69	0/676
2	A	0.35	0/8530	0.59	0/11539
2	B	0.35	0/8496	0.60	4/11495 (0.0%)
All	All	0.35	0/17904	0.60	4/24386 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	558	ALA	N-CA-C	-5.73	95.54	111.00
2	B	660	GLY	N-CA-C	-5.35	99.73	113.10
2	B	444	LEU	CA-CB-CG	5.18	127.22	115.30
2	B	148	ASN	N-CA-C	-5.17	97.04	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	C	390	0	214	12	0
1	D	390	0	214	11	0
2	A	8401	0	8429	258	0
2	B	8367	0	8392	250	0
3	A	135	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	138	0	0	2	0
3	C	5	0	0	0	0
3	D	13	0	0	1	0
All	All	17839	0	17249	517	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 15.

All (517) 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)
2:A:469:GLN:HE22	2:A:557:GLU:H	1.01	1.00
2:A:887:ASN:H	2:A:887:ASN:HD22	1.13	0.95
2:A:144:THR:HG22	2:A:145:PHE:H	1.32	0.95
2:B:469:GLN:HE22	2:B:557:GLU:H	0.99	0.93
2:A:336:GLN:HE21	2:A:417:TYR:H	1.16	0.92
2:B:1072:LYS:HA	2:B:1072:LYS:HE2	1.52	0.91
2:B:364:ALA:H	2:B:384:ASN:HD21	1.18	0.89
2:A:1072:LYS:HE2	2:A:1072:LYS:HA	1.55	0.88
2:B:336:GLN:HE21	2:B:417:TYR:H	1.21	0.85
2:A:790:LEU:O	2:A:795:GLU:HG2	1.76	0.85
2:B:369:LYS:HE3	2:B:371:LEU:HB3	1.58	0.85
2:B:620:MET:HG3	2:B:664:LEU:HD23	1.59	0.84
2:A:360:GLU:HA	2:A:365:GLY:HA3	1.59	0.83
2:B:364:ALA:H	2:B:384:ASN:ND2	1.76	0.83
2:A:665:LYS:HG2	2:A:667:GLY:H	1.46	0.79
2:B:127:ASN:H	2:B:127:ASN:HD22	1.32	0.78
2:B:1059:GLN:HG3	2:B:1060:MET:HE2	1.66	0.77
2:B:723:LYS:HZ2	2:B:723:LYS:HA	1.50	0.77
1:C:4:DT:H5'	2:A:680:SER:HA	1.66	0.77
2:B:372:LEU:HD13	2:B:377:ALA:HB2	1.66	0.77
1:C:5:DC:H2"	1:C:6:DA:H5'	1.67	0.76
2:A:920:ILE:HB	2:A:921:PRO:HD3	1.68	0.76
2:A:863:GLN:HA	2:A:863:GLN:HE21	1.51	0.76
2:B:598:THR:OG1	2:B:601:GLU:HG3	1.86	0.76
2:B:64:SER:OG	2:B:67:ARG:HG2	1.86	0.75
2:B:918:ALA:O	2:B:921:PRO:HD2	1.86	0.75
2:B:309:ILE:HD12	2:B:309:ILE:O	1.87	0.74
1:C:19:DC:H2"	1:C:20:DT:H5'	1.69	0.74
1:D:5:DC:H5'	2:B:921:PRO:HG2	1.68	0.74
2:A:289:THR:O	2:A:293:GLU:HG3	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:190:PRO:HG2	2:A:193:LEU:HB2	1.69	0.74
2:A:998:LYS:HE2	2:A:998:LYS:HA	1.70	0.73
2:A:639:GLN:HE22	2:A:744:THR:HB	1.54	0.73
2:B:725:ALA:HA	2:B:730:HIS:HD2	1.52	0.73
2:B:723:LYS:HZ2	2:B:723:LYS:CA	2.02	0.72
2:B:816:LEU:CD1	2:B:983:VAL:HG21	2.20	0.72
2:B:627:ARG:HH21	2:B:644:LEU:HD12	1.55	0.71
1:D:4:DT:H2"	1:D:5:DC:OP2	1.89	0.71
2:B:373:ASN:HD22	2:B:376:HIS:H	1.35	0.71
2:A:887:ASN:H	2:A:887:ASN:ND2	1.88	0.70
2:B:747:SER:HB3	2:B:765:GLY:HA3	1.72	0.70
2:B:597:LYS:NZ	2:B:602:HIS:HD2	1.90	0.70
2:B:127:ASN:HD22	2:B:127:ASN:N	1.89	0.70
2:B:367:LEU:HD21	2:B:380:LEU:HB2	1.72	0.70
2:A:887:ASN:HD22	2:A:887:ASN:N	1.84	0.69
2:B:496:LYS:HB3	2:B:497:PRO:HD3	1.74	0.69
2:A:369:LYS:C	2:A:371:LEU:H	1.95	0.69
2:B:47:ARG:HD2	2:B:294:ALA:O	1.92	0.69
2:B:721:PHE:O	2:B:723:LYS:HE2	1.94	0.68
2:B:1094:GLU:O	2:B:1095:LEU:HD23	1.93	0.68
2:A:1016:GLN:O	2:A:1020:ALA:HB2	1.94	0.68
1:D:5:DC:H2"	1:D:6:DA:H5'	1.75	0.68
2:B:54:PRO:HG2	2:B:153:GLN:HB2	1.74	0.67
2:A:88:ARG:HG3	2:A:283:PRO:HB2	1.76	0.67
2:A:343:HIS:HE1	2:A:537:GLU:OE2	1.79	0.66
2:A:454:ASN:HD22	2:A:457:ASN:ND2	1.92	0.66
2:B:203:LEU:O	2:B:207:VAL:HG12	1.95	0.66
2:B:469:GLN:HE22	2:B:557:GLU:N	1.83	0.66
2:B:1078:MET:HE2	2:B:1082:GLN:HB3	1.77	0.66
2:B:449:THR:H	2:B:958:ASN:HD21	1.43	0.66
2:A:213:LYS:HE3	2:A:292:GLU:OE1	1.96	0.66
2:A:700:ARG:NH1	2:A:724:GLN:NE2	2.44	0.66
2:B:266:ASN:OD1	2:B:268:LYS:HB2	1.95	0.65
2:A:675:ILE:HD11	2:A:685:ILE:HG12	1.76	0.65
2:A:87:LYS:HE2	2:A:91:GLU:OE1	1.96	0.65
2:B:469:GLN:NE2	2:B:557:GLU:H	1.83	0.65
2:A:645:SER:HA	2:A:656:LEU:HD11	1.78	0.65
2:A:190:PRO:HD2	2:A:193:LEU:HD22	1.79	0.65
2:B:401:VAL:HG12	2:B:408:ILE:HD12	1.78	0.65
2:B:46:SER:O	2:B:49:VAL:HG12	1.95	0.65
2:B:704:VAL:HG23	2:B:719:ALA:HB1	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:178:VAL:HG21	2:A:194:VAL:HA	1.78	0.64
2:A:336:GLN:HE21	2:A:417:TYR:N	1.94	0.64
2:A:633:ASN:OD1	2:A:635:PRO:HG2	1.98	0.64
2:A:454:ASN:HB3	2:A:457:ASN:ND2	2.12	0.64
2:B:710:LYS:O	2:B:711:ASP:HB2	1.96	0.64
2:A:402:ARG:HA	2:A:408:ILE:HG22	1.80	0.64
2:A:639:GLN:NE2	2:A:744:THR:HB	2.12	0.64
2:B:263:ASP:OD1	2:B:265:ASP:HB2	1.97	0.63
2:B:616:THR:CG2	2:B:664:LEU:HB2	2.28	0.63
2:A:469:GLN:HE22	2:A:557:GLU:N	1.86	0.63
2:A:700:ARG:HH12	2:A:724:GLN:NE2	1.96	0.63
2:B:213:LYS:HE3	2:B:292:GLU:OE2	1.96	0.63
2:B:1078:MET:CE	2:B:1082:GLN:HB3	2.29	0.63
2:B:190:PRO:HG2	2:B:193:LEU:HB2	1.80	0.62
2:B:332:LEU:O	2:B:336:GLN:HG3	1.98	0.62
2:A:791:HIS:HA	2:A:795:GLU:HG3	1.80	0.62
2:A:454:ASN:HD21	2:A:456:ASN:HB2	1.63	0.62
2:A:494:ASN:H	2:A:494:ASN:HD22	1.46	0.62
2:B:64:SER:HA	2:B:86:ILE:HD13	1.81	0.61
2:A:127:ASN:N	2:A:127:ASN:HD22	1.97	0.61
2:A:176:LYS:HE3	2:A:176:LYS:HA	1.81	0.61
2:A:364:ALA:H	2:A:384:ASN:ND2	1.99	0.61
2:A:791:HIS:HA	2:A:795:GLU:CG	2.31	0.61
2:B:317:LEU:HG	2:B:318:ARG:NH1	2.16	0.61
2:A:66:ALA:O	2:A:70:LEU:HD23	2.02	0.60
2:A:127:ASN:HD22	2:A:127:ASN:H	1.49	0.60
2:A:257:VAL:HG12	2:A:259:MET:HE3	1.82	0.60
2:A:18:SER:HB2	2:A:139:GLU:OE2	2.02	0.60
2:A:514:ASN:HD22	2:A:514:ASN:H	1.49	0.59
2:A:1005:GLU:O	2:A:1009:LYS:HG3	2.01	0.59
2:B:358:ILE:HD12	2:B:391:TYR:CE1	2.38	0.59
2:B:54:PRO:HG2	2:B:153:GLN:CB	2.32	0.59
2:B:398:ILE:HD12	2:B:399:GLU:N	2.16	0.59
2:B:597:LYS:HZ3	2:B:602:HIS:HD2	1.50	0.59
2:B:715:SER:HB3	2:B:718:MET:CB	2.32	0.59
2:A:570:MET:HG2	2:A:975:TRP:CD2	2.38	0.59
2:A:1075:LEU:HD21	2:A:1086:GLU:HG2	1.85	0.59
2:B:304:PHE:CG	2:B:310:PRO:HG3	2.37	0.58
2:B:810:VAL:O	2:B:814:GLU:HG3	2.02	0.58
2:B:678:TYR:O	2:B:921:PRO:HG3	2.03	0.58
2:B:769:LYS:HB3	2:B:769:LYS:NZ	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:DT:O4	2:A:688:LYS:NZ	2.29	0.58
2:A:369:LYS:O	2:A:371:LEU:N	2.30	0.58
2:A:494:ASN:HD22	2:A:494:ASN:N	2.00	0.58
2:B:398:ILE:HD12	2:B:398:ILE:C	2.24	0.58
2:A:207:VAL:HG11	2:A:905:VAL:HG21	1.86	0.58
2:A:658:GLU:N	2:A:658:GLU:OE1	2.37	0.58
1:C:8:DA:H4'	2:A:886:GLU:O	2.04	0.58
1:D:6:DA:H5'	1:D:6:DA:H8	1.69	0.58
2:A:584:ASN:HA	2:A:587:LYS:HD2	1.86	0.58
2:A:855:THR:OG1	2:A:858:GLU:HG3	2.03	0.58
2:B:15:VAL:HG21	2:B:40:LEU:HD21	1.86	0.58
2:A:393:GLN:HG2	2:A:431:TYR:HB2	1.85	0.57
2:A:653:ASP:OD2	2:A:665:LYS:HD3	2.05	0.57
2:B:191:GLU:HG2	2:B:375:ASN:HB3	1.86	0.57
2:B:343:HIS:CD2	2:B:345:PRO:HD2	2.40	0.57
2:B:367:LEU:O	2:B:369:LYS:N	2.37	0.57
2:A:815:GLN:HE21	2:A:1035:ASN:HB2	1.68	0.57
2:B:633:ASN:OD1	2:B:635:PRO:HG2	2.04	0.57
2:B:654:ILE:HD11	2:B:668:ILE:HD13	1.85	0.57
2:B:725:ALA:HB1	2:B:730:HIS:HB3	1.87	0.57
2:B:848:TRP:CH2	2:B:850:LYS:HA	2.40	0.57
2:A:563:ASN:HD21	2:A:929:ASP:HB3	1.69	0.57
2:A:980:ILE:HG23	2:A:1036:LEU:HD12	1.86	0.57
2:B:262:ILE:HD12	2:B:262:ILE:N	2.19	0.57
1:C:5:DC:H5'	2:A:921:PRO:HG2	1.87	0.57
2:A:870:ALA:HB2	2:A:989:LYS:HD3	1.87	0.57
2:A:795:GLU:HB2	2:A:796:PRO:CD	2.36	0.56
2:A:816:LEU:CD1	2:A:983:VAL:HG21	2.35	0.56
2:A:1004:LEU:HD13	2:A:1025:ILE:HD13	1.85	0.56
2:B:24:ASP:HB3	2:B:27:ALA:HB2	1.87	0.56
2:B:1059:GLN:HG3	2:B:1060:MET:CE	2.34	0.56
2:A:600:ASN:ND2	2:A:600:ASN:H	2.02	0.56
2:B:372:LEU:CD1	2:B:377:ALA:HB2	2.35	0.56
2:B:603:ARG:NH1	2:B:608:ASN:OD1	2.38	0.56
2:A:54:PRO:HG2	2:A:153:GLN:HB2	1.87	0.56
2:A:886:GLU:HG3	2:A:910:TYR:CE2	2.41	0.56
2:B:722:GLY:C	2:B:723:LYS:HZ3	2.09	0.56
2:B:369:LYS:C	2:B:371:LEU:H	2.08	0.56
2:A:82:ASN:HD21	2:A:85:VAL:HG23	1.70	0.56
2:A:858:GLU:O	2:A:862:ILE:HG13	2.05	0.56
2:A:1012:LEU:HD22	2:A:1016:GLN:NE2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:ILE:HB	2:B:235:PRO:HD3	1.88	0.56
2:A:144:THR:HG22	2:A:145:PHE:N	2.12	0.55
2:B:704:VAL:HG13	2:B:705:LEU:H	1.71	0.55
2:B:918:ALA:C	2:B:921:PRO:HD2	2.27	0.55
2:A:465:LEU:HD11	2:A:475:VAL:CG1	2.35	0.55
2:A:444:LEU:N	2:A:444:LEU:HD22	2.22	0.55
2:A:613:GLN:HG2	2:A:666:ARG:HB3	1.87	0.55
2:A:762:THR:HB	2:A:764:THR:HG22	1.89	0.55
2:A:700:ARG:HG3	2:A:700:ARG:HH11	1.70	0.55
2:A:372:LEU:HD12	2:A:372:LEU:O	2.07	0.55
2:B:1072:LYS:HE2	2:B:1072:LYS:CA	2.31	0.55
1:C:11:DA:H5'	2:A:269:THR:O	2.07	0.55
2:A:454:ASN:HB3	2:A:457:ASN:HD21	1.71	0.55
2:B:704:VAL:HG23	2:B:719:ALA:CB	2.36	0.55
2:B:920:ILE:HB	2:B:921:PRO:HD3	1.90	0.54
2:B:303:MET:HE3	2:B:305:PHE:CZ	2.42	0.54
2:B:639:GLN:NE2	2:B:744:THR:HG22	2.23	0.54
2:B:450:LEU:HD11	2:B:957:LEU:HD12	1.89	0.54
2:B:444:LEU:N	2:B:444:LEU:HD22	2.22	0.54
2:A:740:LYS:O	2:A:743:GLU:HB3	2.07	0.54
2:A:936:LEU:HD13	2:A:967:ALA:HA	1.90	0.54
2:A:908:SER:O	2:A:909:ILE:HD12	2.07	0.54
2:A:234:ILE:HB	2:A:235:PRO:HD3	1.90	0.54
2:A:367:LEU:O	2:A:369:LYS:N	2.41	0.53
2:B:100:ALA:O	2:B:104:ARG:HG3	2.08	0.53
2:A:1032:ILE:O	2:A:1036:LEU:HD23	2.09	0.53
2:A:1061:ALA:O	2:A:1062:ALA:CB	2.56	0.53
2:B:639:GLN:NE2	2:B:744:THR:CG2	2.71	0.53
2:A:981:LYS:O	2:A:985:GLU:HG2	2.08	0.53
2:B:355:LYS:O	2:B:359:LEU:HG	2.09	0.53
2:A:422:VAL:HG12	2:A:922:PHE:HA	1.89	0.53
2:A:454:ASN:ND2	2:A:456:ASN:HB2	2.23	0.53
2:A:958:ASN:HD22	2:A:958:ASN:H	1.54	0.53
2:A:336:GLN:NE2	2:A:417:TYR:H	1.96	0.53
2:B:708:ARG:C	2:B:710:LYS:H	2.11	0.53
2:B:1094:GLU:O	2:B:1094:GLU:HG3	2.08	0.53
1:D:4:DT:H5'	2:B:680:SER:HA	1.89	0.53
2:B:995:ASP:CG	2:B:998:LYS:HG2	2.28	0.53
2:B:1086:GLU:OE1	2:B:1089:LYS:HE3	2.09	0.53
2:A:629:ASN:N	2:A:629:ASN:HD22	2.06	0.53
2:B:512:PRO:HB2	2:B:514:ASN:ND2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:204:THR:O	2:A:208:SER:HB2	2.09	0.53
2:A:372:LEU:CD1	2:A:377:ALA:HB2	2.39	0.53
2:B:908:SER:C	2:B:909:ILE:HD12	2.28	0.53
2:A:655:ASN:HB2	2:A:663:GLU:CG	2.39	0.52
2:B:654:ILE:CD1	2:B:668:ILE:HD13	2.39	0.52
2:A:616:THR:O	2:A:620:MET:HG3	2.10	0.52
2:B:20:VAL:HG23	2:B:138:VAL:O	2.08	0.52
2:A:955:ILE:HD13	2:A:963:ALA:HB3	1.90	0.52
2:B:191:GLU:HB2	2:B:375:ASN:HD22	1.74	0.52
2:B:729:ALA:O	2:B:733:GLU:HG3	2.10	0.52
2:B:710:LYS:O	2:B:710:LYS:HG2	2.10	0.52
2:A:369:LYS:C	2:A:371:LEU:N	2.63	0.52
2:B:373:ASN:HD21	2:B:375:ASN:HB2	1.75	0.52
2:B:728:GLU:O	2:B:732:GLU:HB2	2.09	0.52
2:A:262:ILE:HG22	2:A:262:ILE:O	2.09	0.52
2:A:648:ASP:OD2	2:A:655:ASN:HA	2.10	0.52
2:B:597:LYS:HE2	2:B:602:HIS:HB2	1.92	0.52
2:B:653:ASP:O	2:B:665:LYS:HB2	2.09	0.52
2:A:343:HIS:CE1	2:A:537:GLU:OE2	2.61	0.52
2:A:597:LYS:NZ	2:A:602:HIS:HD2	2.07	0.52
2:A:669:ALA:HA	2:A:672:PRO:HG2	1.91	0.52
2:A:72:THR:O	2:A:74:LYS:HG3	2.10	0.51
1:D:6:DA:H5'	1:D:6:DA:C8	2.45	0.51
2:B:635:PRO:HB2	2:B:759:LEU:HD12	1.92	0.51
2:A:793:PHE:O	2:A:796:PRO:HG2	2.10	0.51
2:B:395:PHE:HA	2:B:398:ILE:HG13	1.93	0.51
2:A:37:SER:HB3	2:A:231:THR:HG22	1.93	0.51
2:B:229:GLY:O	2:B:233:GLY:HA3	2.11	0.51
2:B:250:THR:HG22	2:B:250:THR:O	2.10	0.51
2:A:210:LEU:HD22	2:A:214:ILE:HD11	1.92	0.51
2:A:465:LEU:HD11	2:A:475:VAL:HG11	1.92	0.51
2:A:715:SER:HB3	2:A:718:MET:CB	2.40	0.51
2:B:317:LEU:HG	2:B:318:ARG:HH11	1.75	0.51
2:B:367:LEU:HD21	2:B:380:LEU:CB	2.39	0.51
3:D:31:HOH:O	2:B:421:ARG:HG3	2.10	0.51
2:A:863:GLN:HA	2:A:863:GLN:NE2	2.22	0.51
2:B:97:GLU:HG3	3:B:1215:HOH:O	2.11	0.51
2:A:95:HIS:HA	2:B:248:GLU:O	2.11	0.50
2:A:185:ASP:OD2	2:A:188:LEU:HG	2.11	0.50
2:A:262:ILE:O	2:A:263:ASP:HB2	2.11	0.50
2:A:191:GLU:O	2:A:193:LEU:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:257:VAL:HG12	2:A:259:MET:CE	2.41	0.50
2:A:634:MET:N	2:A:635:PRO:HD2	2.26	0.50
2:B:393:GLN:HG2	2:B:431:TYR:HB2	1.93	0.50
2:B:718:MET:HE2	2:B:728:GLU:OE1	2.11	0.50
2:A:887:ASN:ND2	2:A:887:ASN:N	2.54	0.50
1:D:8:DA:H4'	2:B:886:GLU:O	2.11	0.50
2:B:382:GLY:HA2	2:B:385:ARG:HG2	1.92	0.50
2:A:619:LEU:O	2:A:623:LEU:HB2	2.12	0.50
2:A:653:ASP:HB2	2:A:668:ILE:HG23	1.93	0.50
2:B:1053:VAL:HG11	2:B:1075:LEU:HD12	1.92	0.50
2:B:649:LEU:HD13	2:B:737:ARG:NH2	2.27	0.50
2:A:259:MET:HE2	2:A:262:ILE:HD12	1.94	0.49
2:B:465:LEU:HD11	2:B:475:VAL:HG13	1.94	0.49
2:A:783:LYS:O	2:A:786:GLN:HB3	2.12	0.49
2:A:1061:ALA:O	2:A:1062:ALA:HB2	2.12	0.49
2:B:303:MET:HG3	2:B:400:GLN:CD	2.33	0.49
2:B:1048:LYS:HE3	2:B:1048:LYS:HA	1.94	0.49
2:B:81:PHE:CZ	2:B:86:ILE:HG12	2.47	0.49
2:A:88:ARG:HD3	2:A:282:ASP:OD1	2.12	0.49
2:A:717:ALA:HB2	2:A:735:LEU:CD2	2.42	0.49
2:A:1013:GLU:O	2:A:1015:ASP:N	2.46	0.49
2:B:82:ASN:ND2	2:B:85:VAL:H	2.09	0.49
2:A:835:VAL:O	2:A:839:LEU:HG	2.13	0.49
2:A:1014:TYR:HA	2:A:1017:ARG:NE	2.27	0.49
2:B:723:LYS:N	2:B:723:LYS:NZ	2.61	0.49
2:A:134:LEU:HD13	2:A:147:TYR:OH	2.12	0.49
2:B:342:VAL:HG21	2:B:408:ILE:HD11	1.94	0.49
2:A:715:SER:HB3	2:A:718:MET:HB2	1.95	0.49
2:A:1053:VAL:HG11	2:A:1075:LEU:HD12	1.95	0.49
2:B:486:GLU:HG2	2:B:489:LYS:NZ	2.28	0.49
2:B:82:ASN:HD21	2:B:85:VAL:HG23	1.78	0.49
2:B:675:ILE:HD11	2:B:685:ILE:HG12	1.94	0.49
1:D:11:DA:H5'	2:B:269:THR:O	2.13	0.48
2:B:186:GLN:O	2:B:189:LEU:HG	2.13	0.48
2:B:358:ILE:HD12	2:B:391:TYR:HE1	1.74	0.48
2:A:16:TYR:O	2:A:35:LYS:HE2	2.12	0.48
2:B:694:THR:HG21	2:B:782:LEU:HD21	1.96	0.48
2:A:250:THR:O	2:A:250:THR:HG22	2.14	0.48
2:A:430:LYS:HE3	2:A:431:TYR:CE2	2.48	0.48
2:A:1012:LEU:HD11	2:A:1025:ILE:HG22	1.95	0.48
2:A:1041:LEU:O	2:A:1045:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:TYR:O	2:B:35:LYS:CE	2.61	0.48
2:B:207:VAL:HG11	2:B:905:VAL:CG2	2.43	0.48
2:B:886:GLU:HG2	2:B:908:SER:HB3	1.96	0.48
2:A:747:SER:HB3	2:A:765:GLY:HA3	1.94	0.48
2:B:82:ASN:C	2:B:82:ASN:HD22	2.16	0.48
2:B:127:ASN:N	2:B:127:ASN:ND2	2.61	0.48
2:A:590:LEU:HD21	2:A:1050:LEU:HD21	1.96	0.48
2:B:664:LEU:O	2:B:665:LYS:HB2	2.13	0.48
2:A:481:GLU:O	2:A:484:SER:HB3	2.13	0.48
2:B:563:ASN:HD21	2:B:929:ASP:HB3	1.78	0.48
2:B:664:LEU:O	2:B:665:LYS:CB	2.62	0.48
2:B:816:LEU:HD13	2:B:983:VAL:HG21	1.96	0.48
2:B:1094:GLU:C	2:B:1095:LEU:HD23	2.33	0.48
2:A:562:THR:O	2:A:565:PRO:HD2	2.13	0.48
2:B:718:MET:HE1	2:B:728:GLU:HG2	1.94	0.48
2:A:478:MET:O	2:A:600:ASN:HB3	2.14	0.48
2:B:37:SER:HB3	2:B:231:THR:HG22	1.95	0.48
2:B:325:THR:OG1	2:B:328:GLN:HG3	2.14	0.48
2:A:190:PRO:HG3	2:A:262:ILE:HG21	1.95	0.47
2:B:336:GLN:HE21	2:B:417:TYR:N	2.02	0.47
2:B:367:LEU:O	2:B:368:ASN:C	2.52	0.47
2:A:629:ASN:N	2:A:629:ASN:ND2	2.63	0.47
2:B:715:SER:HB3	2:B:718:MET:HB2	1.97	0.47
2:A:467:LEU:O	2:A:471:LEU:HD22	2.15	0.47
2:A:587:LYS:HG2	2:A:609:ASN:O	2.14	0.47
2:B:127:ASN:H	2:B:127:ASN:ND2	2.07	0.47
2:A:256:ILE:N	2:A:256:ILE:HD12	2.29	0.47
2:A:164:LEU:HD22	2:A:284:ILE:HG21	1.95	0.47
2:A:367:LEU:N	2:A:367:LEU:HD12	2.29	0.47
2:B:182:THR:HA	2:B:270:ILE:CD1	2.45	0.47
2:B:1090:LEU:O	2:B:1094:GLU:HB2	2.14	0.47
2:A:671:ASN:N	2:A:672:PRO:HD2	2.28	0.47
2:B:20:VAL:O	2:B:32:ASN:HB2	2.15	0.47
2:B:821:GLN:HE22	2:B:914:GLN:NE2	2.12	0.47
2:A:364:ALA:H	2:A:384:ASN:HD21	1.61	0.47
2:A:446:THR:O	2:A:447:LYS:HB2	2.14	0.47
2:A:969:GLU:O	2:A:973:THR:HG23	2.15	0.47
2:A:1003:ALA:O	2:A:1007:ILE:HG13	2.15	0.47
2:A:1072:LYS:HE2	2:A:1072:LYS:CA	2.35	0.47
2:B:214:ILE:HD11	2:B:242:ILE:HD12	1.95	0.47
2:B:373:ASN:ND2	2:B:375:ASN:HB2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:598:THR:HG1	2:B:601:GLU:HG3	1.76	0.47
2:B:650:PHE:HB3	2:B:696:ALA:CB	2.44	0.47
2:A:347:VAL:HG11	2:A:398:ILE:HD13	1.96	0.47
2:A:665:LYS:HG2	2:A:666:ARG:N	2.29	0.47
2:B:371:LEU:HG	2:B:371:LEU:O	2.15	0.47
1:D:7:DA:C5'	2:B:421:ARG:HE	2.27	0.47
2:A:190:PRO:HG3	2:A:262:ILE:CG2	2.44	0.47
2:A:600:ASN:H	2:A:600:ASN:HD22	1.63	0.47
2:A:769:LYS:HD3	2:A:770:ILE:N	2.29	0.47
2:B:259:MET:HA	2:B:262:ILE:HD13	1.96	0.47
2:B:969:GLU:HG3	2:B:1067:TYR:CE1	2.50	0.47
2:A:657:GLY:O	2:A:659:ASN:N	2.48	0.47
2:A:55:LEU:HB2	2:A:153:GLN:OE1	2.15	0.46
2:A:465:LEU:HD22	2:A:480:ARG:NE	2.30	0.46
2:B:304:PHE:CD2	2:B:310:PRO:HG3	2.50	0.46
2:B:620:MET:CG	2:B:664:LEU:HD23	2.40	0.46
2:B:715:SER:HB3	2:B:718:MET:HB3	1.96	0.46
2:B:995:ASP:OD2	2:B:998:LYS:HG2	2.15	0.46
2:B:741:ASP:O	2:B:745:LEU:HG	2.16	0.46
2:A:89:TYR:O	2:A:93:MET:HG2	2.16	0.46
2:A:514:ASN:H	2:A:514:ASN:ND2	2.13	0.46
2:B:19:LEU:HB3	2:B:32:ASN:ND2	2.30	0.46
2:B:207:VAL:HG11	2:B:905:VAL:HG21	1.97	0.46
2:B:929:ASP:HB2	2:B:950:PHE:O	2.16	0.46
2:A:386:SER:O	2:A:390:SER:HB2	2.15	0.46
2:B:444:LEU:N	2:B:444:LEU:CD2	2.79	0.46
2:B:705:LEU:HD11	2:B:773:LYS:CA	2.45	0.46
2:B:1079:THR:O	2:B:1083:GLN:HG3	2.15	0.46
2:B:669:ALA:HA	2:B:672:PRO:HG2	1.97	0.46
2:A:69:GLU:OE2	2:A:76:THR:HA	2.16	0.46
2:B:715:SER:O	2:B:716:ALA:HB3	2.16	0.46
1:D:7:DA:N6	2:B:318:ARG:HH21	2.14	0.45
2:B:704:VAL:HG13	2:B:705:LEU:N	2.30	0.45
2:A:402:ARG:HA	2:A:408:ILE:CG2	2.45	0.45
2:A:817:GLN:NE2	2:A:818:LYS:N	2.64	0.45
2:B:570:MET:HG2	2:B:975:TRP:CD2	2.51	0.45
2:B:594:SER:HB3	2:B:597:LYS:HB2	1.98	0.45
2:A:432:ASN:HB2	2:A:433:PRO:HD2	1.99	0.45
2:A:598:THR:HG22	2:A:1066:PRO:HD3	1.99	0.45
2:B:440:ARG:O	2:B:444:LEU:HD13	2.17	0.45
2:B:749:VAL:HG13	2:B:762:THR:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:82:ASN:H	2:A:82:ASN:ND2	2.14	0.45
2:A:1053:VAL:O	2:A:1071:GLY:HA3	2.16	0.45
2:B:249:SER:O	2:B:250:THR:HB	2.16	0.45
2:B:371:LEU:HD21	2:B:709:ALA:CB	2.47	0.45
2:A:55:LEU:HG	2:A:153:GLN:HB3	1.98	0.45
2:A:469:GLN:NE2	2:A:557:GLU:H	1.87	0.45
2:A:815:GLN:HE21	2:A:1035:ASN:CB	2.30	0.45
2:B:603:ARG:HH11	2:B:603:ARG:HB3	1.80	0.45
2:B:195:GLU:OE2	2:B:385:ARG:HD3	2.17	0.45
1:C:19:DC:H1'	1:C:20:DT:H5"	1.99	0.45
2:A:421:ARG:HG3	2:A:421:ARG:HH11	1.82	0.45
2:A:708:ARG:HA	2:A:711:ASP:O	2.17	0.45
2:B:343:HIS:HE1	2:B:537:GLU:OE2	2.00	0.45
2:B:598:THR:HG22	2:B:1066:PRO:HD3	1.99	0.45
2:B:797:LEU:O	2:B:801:ILE:HG13	2.17	0.45
2:A:918:ALA:O	2:A:921:PRO:HD2	2.17	0.44
2:B:765:GLY:O	2:B:766:ALA:C	2.55	0.44
2:B:769:LYS:HB3	2:B:769:LYS:HZ3	1.81	0.44
2:B:857:LYS:HE3	2:B:861:ASP:OD2	2.17	0.44
2:A:60:GLN:OE1	2:A:60:GLN:HA	2.16	0.44
2:A:831:PHE:O	2:A:835:VAL:HG23	2.17	0.44
2:A:541:TYR:CE1	2:A:547:LYS:HD3	2.52	0.44
2:B:722:GLY:C	2:B:723:LYS:NZ	2.70	0.44
2:B:328:GLN:HG2	2:B:934:GLN:OE1	2.18	0.44
2:A:259:MET:CE	2:A:259:MET:HA	2.47	0.44
2:B:72:THR:HG22	2:B:294:ALA:HA	2.00	0.44
2:B:355:LYS:HE2	2:B:355:LYS:HB3	1.75	0.44
2:B:368:ASN:HD22	2:B:368:ASN:N	2.16	0.44
2:B:570:MET:HG2	2:B:975:TRP:CG	2.53	0.44
2:B:955:ILE:HD13	2:B:963:ALA:HB3	1.98	0.44
1:C:4:DT:H2"	1:C:5:DC:OP2	2.17	0.44
2:A:657:GLY:O	2:A:660:GLY:N	2.46	0.44
2:A:343:HIS:CG	2:A:553:PRO:HG3	2.52	0.43
2:A:394:LEU:O	2:A:398:ILE:HG23	2.18	0.43
2:A:598:THR:OG1	2:A:601:GLU:HG3	2.18	0.43
2:A:645:SER:HA	2:A:656:LEU:CD1	2.46	0.43
2:A:649:LEU:HD13	2:A:737:ARG:NH2	2.32	0.43
2:A:1016:GLN:H	2:A:1016:GLN:HG3	1.59	0.43
2:A:480:ARG:HH21	2:A:1063:VAL:HG13	1.83	0.43
2:A:1012:LEU:CD1	2:A:1025:ILE:HG22	2.49	0.43
2:B:597:LYS:HZ3	2:B:602:HIS:CD2	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:95:HIS:NE2	2:A:251:ASP:OD2	2.42	0.43
2:A:19:LEU:HB3	2:A:32:ASN:ND2	2.34	0.43
2:A:175:ALA:HB1	2:A:186:GLN:HG3	2.01	0.43
2:B:185:ASP:OD2	2:B:186:GLN:N	2.52	0.43
2:B:718:MET:CE	2:B:728:GLU:HG2	2.49	0.43
2:B:1075:LEU:HD21	2:B:1086:GLU:HG2	2.01	0.43
2:A:64:SER:OG	2:A:67:ARG:HG3	2.19	0.43
2:A:384:ASN:HD22	2:A:384:ASN:HA	1.60	0.43
2:B:126:ALA:C	2:B:128:ARG:H	2.22	0.43
1:D:7:DA:C5	2:B:318:ARG:NE	2.87	0.43
2:A:514:ASN:HD22	2:A:514:ASN:N	2.09	0.43
2:A:694:THR:HG22	2:A:777:ILE:HD12	2.01	0.43
2:A:815:GLN:NE2	2:A:1035:ASN:HB2	2.33	0.43
2:B:319:ASN:HD22	2:B:319:ASN:HA	1.49	0.43
2:B:366:THR:O	2:B:366:THR:HG22	2.19	0.43
2:B:369:LYS:C	2:B:371:LEU:N	2.72	0.43
2:A:465:LEU:HD11	2:A:475:VAL:HG13	2.01	0.43
2:B:1061:ALA:O	2:B:1062:ALA:HB2	2.19	0.43
2:B:1093:GLU:C	2:B:1095:LEU:H	2.22	0.43
2:A:82:ASN:HD22	2:A:82:ASN:C	2.21	0.42
2:A:259:MET:HE2	2:A:259:MET:HA	2.01	0.42
2:A:717:ALA:HB2	2:A:735:LEU:HD22	1.99	0.42
2:A:762:THR:CB	2:A:764:THR:HG22	2.47	0.42
2:A:795:GLU:HB2	2:A:796:PRO:HD3	2.01	0.42
2:B:309:ILE:HD12	2:B:309:ILE:C	2.37	0.42
2:B:369:LYS:HE3	2:B:371:LEU:HD23	2.01	0.42
2:B:376:HIS:O	2:B:380:LEU:HG	2.18	0.42
2:B:470:ALA:HB3	2:B:534:ALA:HB2	2.01	0.42
2:A:565:PRO:HA	2:A:677:ILE:HG12	2.01	0.42
2:A:700:ARG:NH1	2:A:724:GLN:HE21	2.15	0.42
2:B:364:ALA:O	2:B:365:GLY:O	2.37	0.42
2:B:422:VAL:O	2:B:926:GLY:HA2	2.19	0.42
2:B:621:GLU:HA	2:B:621:GLU:OE1	2.19	0.42
2:B:650:PHE:HB3	2:B:696:ALA:HB1	2.00	0.42
2:A:850:LYS:HD2	2:A:850:LYS:O	2.19	0.42
2:B:335:GLU:OE2	2:B:937:SER:HB3	2.19	0.42
2:B:869:LEU:HD21	3:B:1201:HOH:O	2.19	0.42
2:B:501:MET:HE1	2:B:519:LEU:HG	2.01	0.42
2:A:144:THR:CG2	2:A:145:PHE:H	2.13	0.42
2:A:791:HIS:HA	2:A:795:GLU:HG2	2.01	0.42
2:B:447:LYS:HE2	2:B:447:LYS:HB3	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:721:PHE:HB3	2:B:734:LEU:CD1	2.49	0.42
2:A:54:PRO:HG2	2:A:153:GLN:CB	2.49	0.42
2:A:749:VAL:HG11	2:A:784:ALA:HA	2.02	0.42
2:B:58:VAL:HG21	2:B:157:LEU:HD13	2.02	0.42
2:B:319:ASN:N	2:B:320:PRO:HD3	2.33	0.42
2:A:16:TYR:O	2:A:35:LYS:CE	2.68	0.42
2:A:134:LEU:O	2:A:137:ILE:HG12	2.20	0.42
2:A:177:ASP:O	2:A:181:ILE:HG13	2.20	0.42
2:A:837:GLU:O	2:A:840:ALA:HB3	2.19	0.42
2:A:932:MET:CE	2:A:1060:MET:SD	3.07	0.42
2:A:444:LEU:N	2:A:444:LEU:CD2	2.81	0.42
2:A:651:LEU:HA	2:A:652:PRO:HD3	1.87	0.42
2:B:783:LYS:O	2:B:787:GLU:HG3	2.19	0.42
1:C:5:DC:C2'	1:C:6:DA:H5'	2.45	0.42
2:A:648:ASP:HB2	2:A:656:LEU:HG	2.01	0.42
2:A:662:LEU:HD23	2:A:662:LEU:O	2.20	0.42
2:B:144:THR:HB	2:B:145:PHE:H	1.52	0.42
2:B:651:LEU:HA	2:B:652:PRO:HD3	1.88	0.42
2:B:1015:ASP:OD1	2:B:1016:GLN:HG3	2.19	0.42
2:A:195:GLU:O	2:A:199:THR:HG22	2.19	0.42
2:A:443:ILE:C	2:A:444:LEU:HD22	2.41	0.42
2:A:512:PRO:HB2	2:A:514:ASN:ND2	2.35	0.42
2:B:693:VAL:O	2:B:697:ILE:HG13	2.20	0.42
2:B:705:LEU:HD11	2:B:773:LYS:HA	2.01	0.42
2:A:655:ASN:HB2	2:A:663:GLU:HG3	2.02	0.41
2:B:705:LEU:HG	2:B:772:PRO:HB2	2.01	0.41
2:A:111:LEU:HD13	2:A:144:THR:HG22	2.01	0.41
2:A:196:GLN:O	2:A:199:THR:HG22	2.20	0.41
2:A:585:ILE:HD12	2:A:585:ILE:HA	1.95	0.41
2:A:90:LYS:O	2:A:94:GLU:HG3	2.21	0.41
2:A:700:ARG:HH11	2:A:700:ARG:CG	2.33	0.41
2:A:815:GLN:NE2	2:A:1035:ASN:CB	2.83	0.41
2:B:496:LYS:HE2	2:B:500:ASP:OD1	2.20	0.41
2:A:191:GLU:C	2:A:193:LEU:H	2.22	0.41
2:A:372:LEU:HB2	2:A:702:SER:OG	2.21	0.41
2:A:769:LYS:HD3	2:A:769:LYS:C	2.40	0.41
2:B:26:LYS:HG2	2:B:847:THR:HG21	2.02	0.41
2:B:398:ILE:HD13	2:B:402:ARG:CZ	2.50	0.41
2:B:730:HIS:O	2:B:734:LEU:HG	2.20	0.41
1:C:7:DA:OP1	2:A:318:ARG:NH1	2.54	0.41
2:A:263:ASP:HA	2:A:264:PRO:HD2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:450:LEU:HD11	2:A:957:LEU:HD12	2.02	0.41
2:A:463:PHE:HA	2:A:957:LEU:HD13	2.01	0.41
2:A:494:ASN:N	2:A:494:ASN:ND2	2.66	0.41
2:A:616:THR:CG2	2:A:664:LEU:HB2	2.51	0.41
2:A:644:LEU:HB3	2:A:656:LEU:HD21	2.03	0.41
2:A:706:LYS:O	2:A:706:LYS:HG3	2.19	0.41
2:A:438:LEU:C	2:A:438:LEU:HD23	2.40	0.41
2:B:514:ASN:C	2:B:514:ASN:HD22	2.23	0.41
2:B:708:ARG:C	2:B:710:LYS:N	2.73	0.41
2:B:773:LYS:O	2:B:773:LYS:HG3	2.19	0.41
2:B:778:LYS:HA	2:B:778:LYS:HD3	1.87	0.41
2:A:88:ARG:CD	2:A:283:PRO:HD2	2.51	0.41
2:A:454:ASN:HD22	2:A:457:ASN:HD21	1.66	0.41
2:B:249:SER:O	2:B:250:THR:CB	2.69	0.41
2:B:1088:ASN:O	2:B:1091:PHE:HB3	2.21	0.41
1:C:21:DT:C4	1:C:22:DC:N4	2.88	0.41
2:A:82:ASN:ND2	2:A:85:VAL:HG23	2.35	0.41
2:A:620:MET:HG2	2:A:664:LEU:HD12	2.02	0.41
2:A:721:PHE:HB3	2:A:734:LEU:HD12	2.03	0.41
2:B:185:ASP:OD2	2:B:185:ASP:C	2.59	0.41
2:B:443:ILE:C	2:B:444:LEU:HD22	2.41	0.41
2:B:875:THR:HG22	2:B:982:ASN:ND2	2.36	0.41
2:B:1075:LEU:HD22	2:B:1078:MET:SD	2.61	0.41
2:A:127:ASN:H	2:A:127:ASN:ND2	2.17	0.41
2:B:797:LEU:O	2:B:797:LEU:HD12	2.21	0.41
2:B:936:LEU:HD21	2:B:953:MET:CE	2.51	0.41
2:A:465:LEU:N	2:A:483:MET:HE1	2.36	0.40
2:A:302:LYS:HD2	2:A:304:PHE:CE1	2.56	0.40
2:A:373:ASN:HD22	2:A:376:HIS:H	1.69	0.40
2:A:134:LEU:HD23	2:A:134:LEU:HA	1.94	0.40
2:B:585:ILE:HG12	2:B:590:LEU:HD23	2.03	0.40
2:B:720:MET:SD	2:B:721:PHE:CE1	3.14	0.40
2:A:644:LEU:HD23	2:A:644:LEU:HA	1.94	0.40
2:B:819:ALA:HB2	2:B:1036:LEU:HD21	2.03	0.40
2:B:886:GLU:HA	2:B:909:ILE:O	2.22	0.40
2:B:960:ILE:HB	2:B:1063:VAL:HG21	2.04	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	
2	A	1087/1117 (97%)	1024 (94%)	50 (5%)	13 (1%)	13	19
2	B	1083/1117 (97%)	1026 (95%)	43 (4%)	14 (1%)	12	17
All	All	2170/2234 (97%)	2050 (94%)	93 (4%)	27 (1%)	13	19

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	191	GLU
2	A	658	GLU
2	A	1014	TYR
2	A	1062	ALA
2	B	191	GLU
2	B	365	GLY
2	B	368	ASN
2	B	664	LEU
2	B	665	LYS
2	B	711	ASP
2	B	1062	ALA
2	A	192	GLY
2	A	365	GLY
2	A	368	ASN
2	A	370	GLU
2	A	633	ASN
2	B	366	THR
2	B	764	THR
2	A	263	ASP
2	B	715	SER
2	A	775	TYR
2	B	666	ARG
2	B	1094	GLU
2	A	366	THR
2	B	370	GLU

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Mol	Chain	Res	Type
2	A	711	ASP
2	B	445	PRO

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	
2	A	910/934 (97%)	867 (95%)	43 (5%)	26	42
2	B	907/934 (97%)	870 (96%)	37 (4%)	30	48
All	All	1817/1868 (97%)	1737 (96%)	80 (4%)	28	45

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	49	VAL
2	A	52	GLU
2	A	82	ASN
2	A	127	ASN
2	A	163	ARG
2	A	210	LEU
2	A	255	ASN
2	A	265	ASP
2	A	266	ASN
2	A	292	GLU
2	A	302	LYS
2	A	309	ILE
2	A	319	ASN
2	A	372	LEU
2	A	444	LEU
2	A	471	LEU
2	A	472	ASP
2	A	483	MET
2	A	494	ASN
2	A	514	ASN
2	A	541	TYR

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Mol	Chain	Res	Type
2	A	603	ARG
2	A	623	LEU
2	A	634	MET
2	A	662	LEU
2	A	700	ARG
2	A	723	LYS
2	A	760	GLN
2	A	771	ASN
2	A	817	GLN
2	A	838	LYS
2	A	863	GLN
2	A	869	LEU
2	A	886	GLU
2	A	887	ASN
2	A	892	ASN
2	A	944	LYS
2	A	958	ASN
2	A	973	THR
2	A	1004	LEU
2	A	1034	ARG
2	A	1038	ASN
2	A	1041	LEU
2	B	82	ASN
2	B	127	ASN
2	B	144	THR
2	B	163	ARG
2	B	191	GLU
2	B	228	LEU
2	B	265	ASP
2	B	319	ASN
2	B	370	GLU
2	B	372	LEU
2	B	384	ASN
2	B	402	ARG
2	B	430	LYS
2	B	444	LEU
2	B	471	LEU
2	B	483	MET
2	B	489	LYS
2	B	514	ASN
2	B	520	ASN
2	B	580	ASP

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Mol	Chain	Res	Type
2	B	603	ARG
2	B	605	THR
2	B	623	LEU
2	B	662	LEU
2	B	664	LEU
2	B	683	ARG
2	B	688	LYS
2	B	723	LYS
2	B	728	GLU
2	B	771	ASN
2	B	773	LYS
2	B	817	GLN
2	B	838	LYS
2	B	892	ASN
2	B	907	MET
2	B	1036	LEU
2	B	1041	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	82	ASN
2	A	127	ASN
2	A	150	GLN
2	A	186	GLN
2	A	255	ASN
2	A	266	ASN
2	A	298	ASN
2	A	316	GLN
2	A	319	ASN
2	A	324	ASN
2	A	336	GLN
2	A	343	HIS
2	A	348	GLN
2	A	368	ASN
2	A	373	ASN
2	A	376	HIS
2	A	384	ASN
2	A	393	GLN
2	A	414	HIS
2	A	454	ASN
2	A	455	GLN

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Mol	Chain	Res	Type
2	A	456	ASN
2	A	457	ASN
2	A	469	GLN
2	A	494	ASN
2	A	514	ASN
2	A	563	ASN
2	A	600	ASN
2	A	602	HIS
2	A	629	ASN
2	A	639	GLN
2	A	724	GLN
2	A	771	ASN
2	A	781	GLN
2	A	815	GLN
2	A	817	GLN
2	A	833	GLN
2	A	863	GLN
2	A	887	ASN
2	A	892	ASN
2	A	914	GLN
2	A	954	ASN
2	A	958	ASN
2	A	982	ASN
2	A	1016	GLN
2	A	1035	ASN
2	A	1059	GLN
2	A	1070	ASN
2	B	82	ASN
2	B	127	ASN
2	B	150	GLN
2	B	255	ASN
2	B	298	ASN
2	B	314	ASN
2	B	316	GLN
2	B	319	ASN
2	B	324	ASN
2	B	336	GLN
2	B	343	HIS
2	B	348	GLN
2	B	368	ASN
2	B	373	ASN
2	B	375	ASN

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Mol	Chain	Res	Type
2	B	384	ASN
2	B	414	HIS
2	B	455	GLN
2	B	457	ASN
2	B	469	GLN
2	B	506	ASN
2	B	514	ASN
2	B	520	ASN
2	B	563	ASN
2	B	602	HIS
2	B	613	GLN
2	B	629	ASN
2	B	639	GLN
2	B	655	ASN
2	B	724	GLN
2	B	730	HIS
2	B	771	ASN
2	B	786	GLN
2	B	815	GLN
2	B	817	GLN
2	B	878	GLN
2	B	892	ASN
2	B	893	GLN
2	B	914	GLN
2	B	954	ASN
2	B	958	ASN
2	B	982	ASN
2	B	1035	ASN
2	B	1047	HIS
2	B	1059	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	C	19/33 (57%)	-0.22	1 (5%) 26 25	25, 31, 59, 62	0
1	D	19/33 (57%)	-0.41	0 100 100	18, 28, 51, 59	0
2	A	1089/1117 (97%)	-0.17	27 (2%) 57 55	8, 24, 50, 66	0
2	B	1085/1117 (97%)	-0.24	25 (2%) 60 58	9, 22, 49, 67	0
All	All	2212/2300 (96%)	-0.21	53 (2%) 59 57	8, 23, 50, 67	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	368	ASN	7.4
2	B	368	ASN	5.7
2	A	1014	TYR	5.6
2	B	724	GLN	5.2
2	B	1014	TYR	4.8
2	A	1019	ASN	3.9
2	A	1015	ASP	3.7
2	B	725	ALA	3.7
2	A	657	GLY	3.5
2	B	664	LEU	3.4
2	A	712	PRO	3.4
2	B	726	ALA	3.3
2	B	713	ASN	3.2
2	A	724	GLN	3.2
2	A	658	GLU	3.2
2	B	712	PRO	3.0
2	B	1018	GLU	3.0
2	A	727	SER	3.0
2	A	1013	GLU	2.9
2	A	29	GLY	2.8
2	B	709	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
2	A	754	LYS	2.8
2	B	769	LYS	2.7
2	A	406	GLU	2.7
2	A	730	HIS	2.7
2	B	708	ARG	2.7
2	B	710	LYS	2.7
2	B	369	LYS	2.6
2	B	754	LYS	2.5
2	A	366	THR	2.5
2	B	42	GLU	2.4
2	B	1070	ASN	2.4
2	A	28	GLU	2.4
2	B	1015	ASP	2.4
2	A	729	ALA	2.4
2	A	267	LYS	2.4
2	A	726	ALA	2.4
2	A	42	GLU	2.3
2	B	265	ASP	2.3
1	C	4	DT	2.3
2	B	722	GLY	2.3
2	B	714	ILE	2.2
2	B	70	LEU	2.2
2	A	1098	ARG	2.2
2	A	631	ALA	2.2
2	B	1019	ASN	2.2
2	A	369	LYS	2.1
2	A	844	LYS	2.1
2	B	264	PRO	2.1
2	A	713	ASN	2.1
2	A	199	THR	2.0
2	B	263	ASP	2.0
2	A	659	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.