Full wwPDB X-ray Structure Validation Report ⓘ

Feb 11, 2024 – 09:36 AM EST

PDB ID	:	3C2P
Title	:	X-ray crystal structure of the N4 mini-vRNAP P1 promoter complex
Authors	:	Gleghorn, M.L.; Murakami, K.S.
Deposited on	:	2008-01-25
Resolution	:	2.00 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:

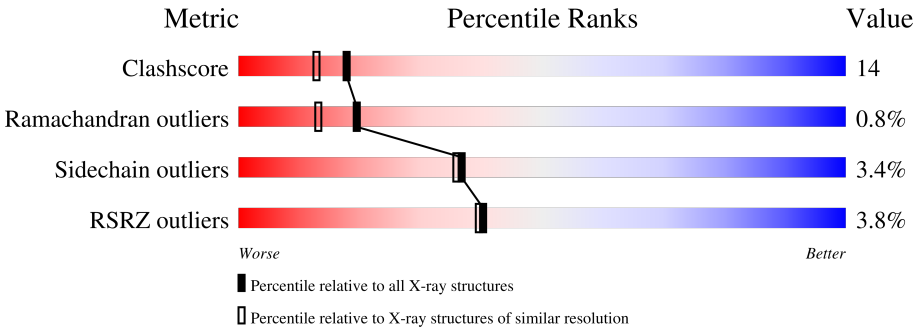
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.00 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	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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%, 39%, 21%, 39%
1	D	33	39%, 18%, 42%
2	A	1117	4%, 72%, 23%
2	B	1117	3%, 72%, 24%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18317 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 P1 Promoter DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	20	Total	C	N	O	P	0	0	0
			411	196	83	113	19			
1	D	19	Total	C	N	O	P	0	0	0
			389	186	78	107	18			

- Molecule 2 is a protein called Virion RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1093	Total	C	N	O	S	0	0	0
			8431	5293	1433	1664	41			
2	B	1093	Total	C	N	O	S	0	0	0
			8436	5296	1433	1666	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.

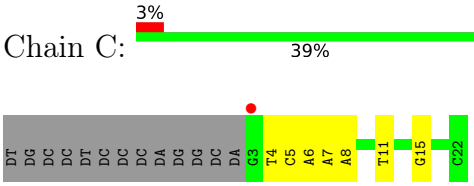
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	14	Total O 14 14	0	0
3	D	24	Total O 24 24	0	0
3	A	292	Total O 292 292	0	0
3	B	320	Total O 320 320	0	0

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.

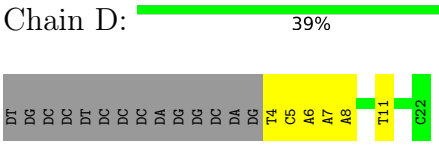
• Molecule 1: P1 Promoter DNA

Chain C:



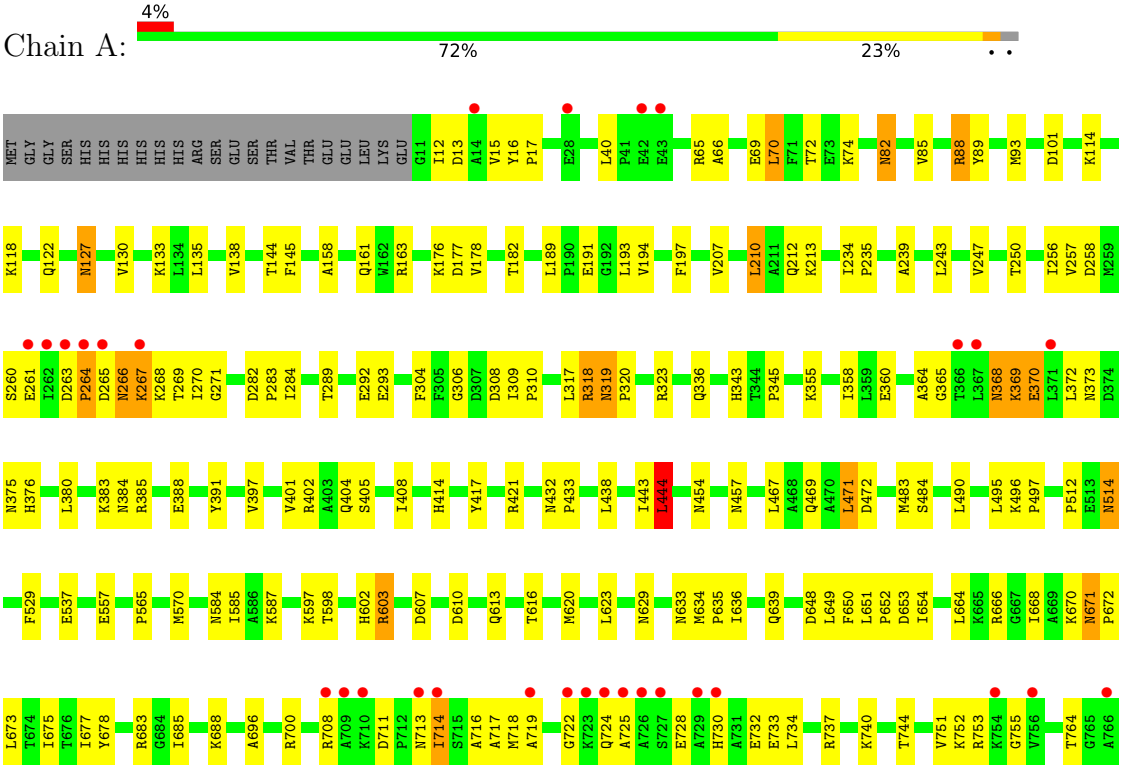
• Molecule 1: P1 Promoter DNA

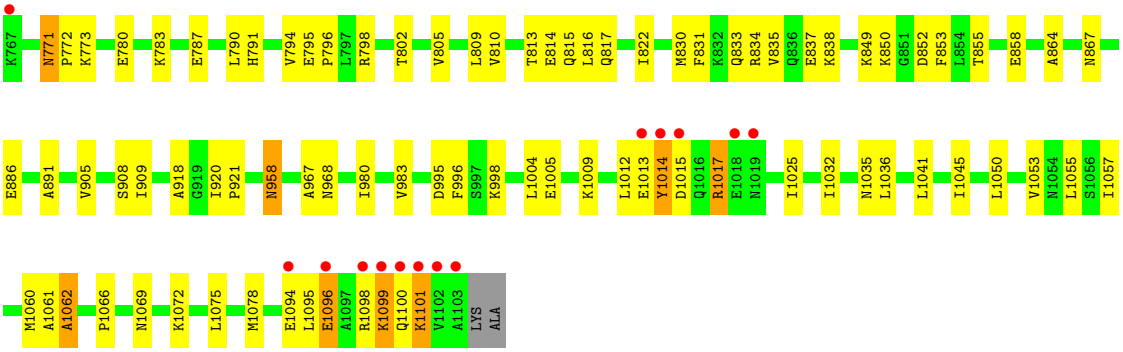
Chain D:



• Molecule 2: Virion RNA polymerase

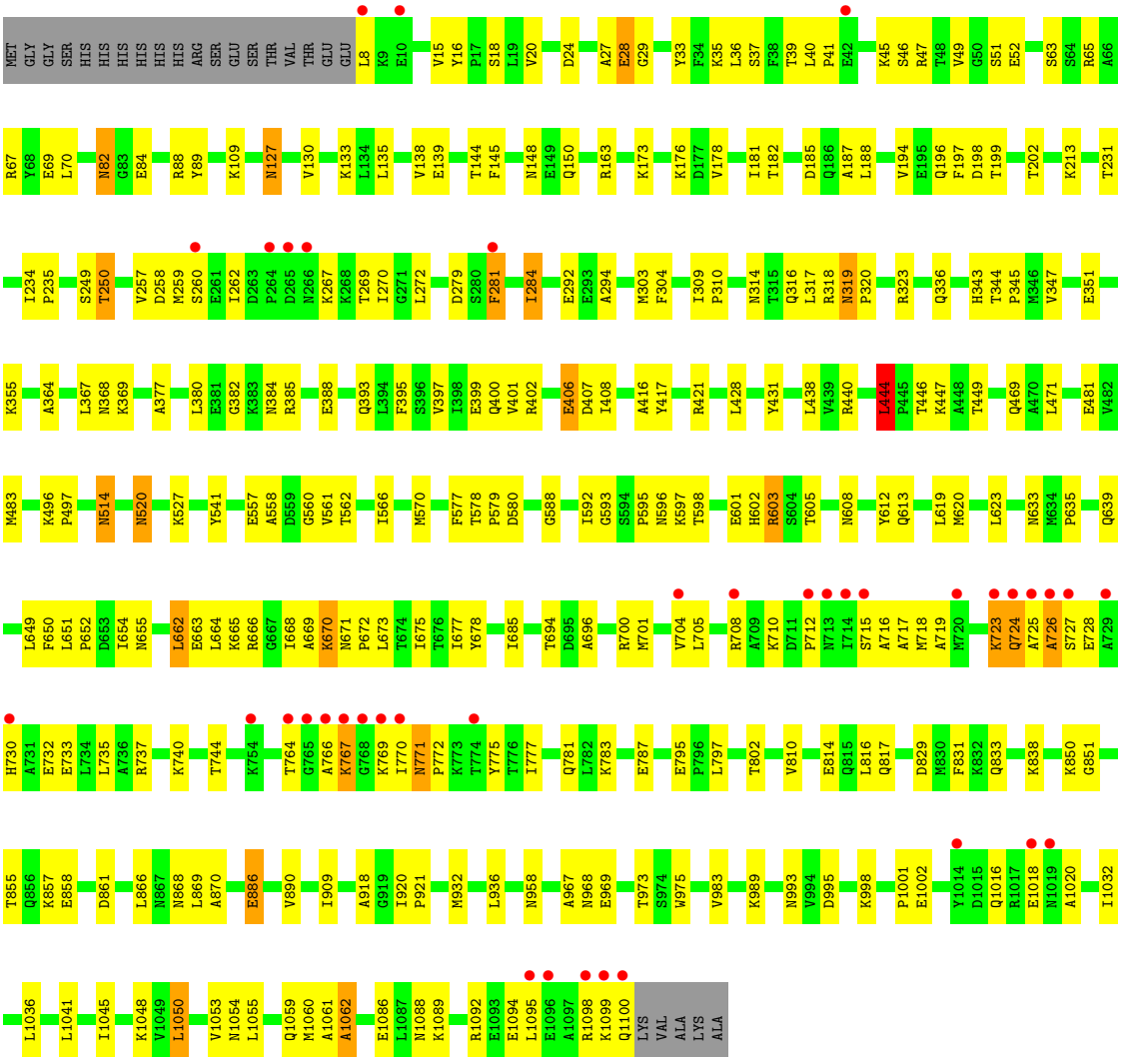
Chain A:





• 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	81.46Å 111.19Å 276.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 45.92 – 2.00	Depositor EDS
% Data completeness (in resolution range)	83.1 (50.00-2.00) 83.6 (45.92-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.256 0.219 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	20.8	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.4	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	0.93	EDS
Total number of atoms	18317	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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	0.32	0/463	0.76	0/713
1	D	0.30	0/438	0.75	0/674
2	A	0.33	0/8560	0.58	2/11579 (0.0%)
2	B	0.34	0/8565	0.59	3/11585 (0.0%)
All	All	0.33	0/18026	0.60	5/24551 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	444	LEU	CA-CB-CG	7.58	132.73	115.30
2	A	444	LEU	CA-CB-CG	5.80	128.65	115.30
2	B	558	ALA	N-CA-C	-5.11	97.19	111.00
2	A	852	ASP	N-CA-C	-5.02	97.44	111.00
2	B	148	ASN	N-CA-C	-5.01	97.47	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	411	0	225	7	0
1	D	389	0	214	8	0
2	A	8431	0	8464	259	0
2	B	8436	0	8467	215	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	292	0	0	2	0
3	B	320	0	0	0	0
3	C	14	0	0	0	0
3	D	24	0	0	0	0
All	All	18317	0	17370	478	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 14.

All (478) 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:B:144:THR:HG22	2:B:145:PHE:H	1.17	1.09
2:A:161:GLN:HB3	2:A:213:LYS:NZ	1.71	1.03
2:B:1059:GLN:HG3	2:B:1060:MET:HE2	1.40	1.00
2:B:469:GLN:HE22	2:B:557:GLU:H	1.02	0.97
2:A:469:GLN:HE22	2:A:557:GLU:H	1.01	0.96
2:A:364:ALA:H	2:A:384:ASN:ND2	1.65	0.93
2:A:158:ALA:HA	2:A:213:LYS:NZ	1.82	0.93
2:B:24:ASP:HB3	2:B:27:ALA:HB2	1.50	0.93
2:A:336:GLN:HE21	2:A:417:TYR:H	1.13	0.92
2:B:336:GLN:HE21	2:B:417:TYR:H	1.17	0.92
2:B:700:ARG:NH2	2:B:723:LYS:HD2	1.85	0.92
2:A:158:ALA:HA	2:A:213:LYS:HZ3	1.33	0.91
2:A:161:GLN:HB3	2:A:213:LYS:HZ1	1.29	0.91
2:A:364:ALA:H	2:A:384:ASN:HD21	1.16	0.90
2:B:364:ALA:H	2:B:384:ASN:HD21	1.22	0.88
2:A:584:ASN:HA	2:A:587:LYS:HD2	1.57	0.87
2:A:700:ARG:HH22	2:A:724:GLN:NE2	1.72	0.85
2:B:364:ALA:H	2:B:384:ASN:ND2	1.77	0.83
2:A:127:ASN:HD22	2:A:127:ASN:H	1.23	0.83
2:B:601:GLU:O	2:B:605:THR:HG22	1.78	0.82
2:B:267:LYS:HE2	2:B:267:LYS:HA	1.63	0.79
2:A:958:ASN:HD22	2:A:958:ASN:H	1.27	0.79
2:A:714:ILE:HG23	2:A:719:ALA:HB2	1.66	0.78
2:A:161:GLN:CB	2:A:213:LYS:HZ1	1.95	0.77
2:B:395:PHE:O	2:B:399:GLU:HG3	1.85	0.76
1:C:8:DA:H4'	2:A:886:GLU:O	1.86	0.75
2:B:723:LYS:O	2:B:724:GLN:HB2	1.87	0.75
2:B:249:SER:O	2:B:250:THR:HG22	1.86	0.75
2:B:449:THR:H	2:B:958:ASN:HD21	1.31	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:THR:HG22	2:B:145:PHE:N	1.99	0.74
2:A:752:LYS:NZ	2:A:755:GLY:HA2	2.01	0.73
2:B:127:ASN:H	2:B:127:ASN:HD22	1.35	0.73
2:A:368:ASN:O	2:A:370:GLU:N	2.21	0.73
2:A:675:ILE:HD11	2:A:685:ILE:HG12	1.69	0.73
2:A:671:ASN:HB3	2:A:672:PRO:HD3	1.69	0.73
2:A:82:ASN:HD22	2:A:82:ASN:C	1.92	0.72
2:B:496:LYS:HB3	2:B:497:PRO:HD3	1.70	0.72
2:B:613:GLN:HG2	2:B:666:ARG:HD2	1.72	0.72
2:A:920:ILE:HB	2:A:921:PRO:HD3	1.72	0.72
2:A:855:THR:OG1	2:A:858:GLU:HG3	1.88	0.71
2:B:995:ASP:CG	2:B:998:LYS:HG2	2.11	0.71
2:B:1032:ILE:O	2:B:1036:LEU:HD13	1.91	0.71
2:A:364:ALA:N	2:A:384:ASN:HD21	1.89	0.70
2:A:790:LEU:O	2:A:795:GLU:HG2	1.91	0.70
2:B:1045:ILE:HG23	2:B:1094:GLU:HG2	1.74	0.70
2:B:46:SER:O	2:B:49:VAL:HG12	1.92	0.69
2:B:603:ARG:NH1	2:B:608:ASN:OD1	2.26	0.69
1:D:4:DT:H2"	1:D:5:DC:OP2	1.92	0.69
2:B:597:LYS:NZ	2:B:602:HIS:HD2	1.90	0.69
2:B:655:ASN:HB2	2:B:663:GLU:HB3	1.75	0.68
2:A:267:LYS:HD3	2:A:267:LYS:H	1.58	0.68
2:A:810:VAL:O	2:A:814:GLU:HG3	1.94	0.68
2:A:1032:ILE:O	2:A:1036:LEU:HD23	1.95	0.67
2:A:266:ASN:ND2	2:A:268:LYS:H	1.93	0.66
2:B:705:LEU:HD21	2:B:772:PRO:HG2	1.78	0.66
2:A:469:GLN:NE2	2:A:557:GLU:H	1.85	0.66
2:A:178:VAL:HG21	2:A:194:VAL:HA	1.76	0.66
2:A:15:VAL:C	2:A:17:PRO:HD3	2.17	0.66
2:A:161:GLN:HB3	2:A:213:LYS:CE	2.25	0.66
2:A:127:ASN:HD22	2:A:127:ASN:N	1.93	0.65
2:A:718:MET:SD	2:A:722:GLY:HA2	2.37	0.65
2:B:715:SER:HB3	2:B:718:MET:HB2	1.77	0.65
2:B:918:ALA:O	2:B:921:PRO:HD2	1.95	0.65
2:A:469:GLN:HE22	2:A:557:GLU:N	1.86	0.65
2:B:654:ILE:C	2:B:655:ASN:HD22	2.01	0.65
2:A:402:ARG:HA	2:A:408:ILE:HG22	1.78	0.64
2:B:728:GLU:O	2:B:732:GLU:HB2	1.98	0.64
2:B:1001:PRO:HG2	2:B:1002:GLU:OE2	1.96	0.64
2:B:920:ILE:HB	2:B:921:PRO:HD3	1.80	0.64
2:B:469:GLN:NE2	2:B:557:GLU:H	1.86	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:597:LYS:NZ	2:A:602:HIS:HD2	1.95	0.63
2:B:185:ASP:OD2	2:B:188:LEU:HG	1.98	0.63
2:B:1095:LEU:O	2:B:1098:ARG:HB3	1.98	0.63
2:B:816:LEU:CD1	2:B:983:VAL:HG21	2.29	0.63
2:A:318:ARG:HB3	2:A:421:ARG:HH12	1.63	0.62
2:A:250:THR:O	2:A:250:THR:HG22	2.00	0.62
2:A:968:ASN:HD21	2:A:1060:MET:H	1.48	0.62
1:D:5:DC:H5'	2:B:921:PRO:HG2	1.81	0.61
2:B:725:ALA:O	2:B:726:ALA:CB	2.49	0.60
2:A:634:MET:HB3	2:A:635:PRO:HD3	1.84	0.60
2:B:284:ILE:HD13	2:B:284:ILE:O	2.01	0.60
2:A:708:ARG:HH21	2:A:716:ALA:HA	1.65	0.60
2:A:1095:LEU:O	2:A:1099:LYS:HB2	2.01	0.60
2:A:1100:GLN:O	2:A:1101:LYS:HG3	2.01	0.60
2:B:89:TYR:CZ	2:B:284:ILE:HD11	2.36	0.59
2:B:671:ASN:HB3	2:B:672:PRO:HD3	1.84	0.59
2:A:610:ASP:HB2	3:A:1110:HOH:O	2.02	0.59
2:A:88:ARG:HD3	2:A:282:ASP:OD1	2.01	0.59
2:B:402:ARG:HG3	2:B:408:ILE:HD12	1.85	0.59
2:B:810:VAL:O	2:B:814:GLU:HG3	2.03	0.59
2:A:613:GLN:HG2	2:A:666:ARG:HB3	1.85	0.59
2:A:16:TYR:N	2:A:17:PRO:HD3	2.18	0.58
2:A:1050:LEU:O	2:A:1055:LEU:HD21	2.03	0.58
2:A:918:ALA:O	2:A:921:PRO:HD2	2.03	0.58
2:B:678:TYR:O	2:B:921:PRO:HG3	2.03	0.58
2:A:454:ASN:HD22	2:A:457:ASN:ND2	2.01	0.58
2:A:317:LEU:HD21	2:A:318:ARG:NH2	2.19	0.58
2:B:127:ASN:HD22	2:B:127:ASN:N	2.02	0.57
2:B:317:LEU:HG	2:B:318:ARG:NH1	2.20	0.57
2:A:1014:TYR:HA	2:A:1017:ARG:HD3	1.84	0.57
2:B:649:LEU:HD13	2:B:737:ARG:NH2	2.19	0.57
2:A:158:ALA:HA	2:A:213:LYS:HZ2	1.68	0.57
2:A:598:THR:HG22	2:A:1066:PRO:HD3	1.86	0.57
2:B:726:ALA:O	2:B:730:HIS:HB3	2.04	0.57
2:A:266:ASN:HD22	2:A:267:LYS:N	2.01	0.57
2:B:33:TYR:HA	2:B:36:LEU:HB2	1.86	0.57
2:A:751:VAL:HG12	2:A:753:ARG:HG2	1.87	0.57
2:B:730:HIS:HA	2:B:733:GLU:OE2	2.04	0.57
2:B:769:LYS:HE3	2:B:770:ILE:H	1.69	0.57
2:B:783:LYS:O	2:B:787:GLU:HG2	2.04	0.57
2:A:1013:GLU:O	2:A:1015:ASP:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:397:VAL:O	2:B:401:VAL:HG23	2.05	0.57
2:B:469:GLN:HE22	2:B:557:GLU:N	1.86	0.57
2:B:725:ALA:O	2:B:726:ALA:HB3	2.05	0.57
1:D:11:DT:H5'	2:B:269:THR:O	2.04	0.56
2:B:671:ASN:O	2:B:675:ILE:HG12	2.05	0.56
2:A:496:LYS:HB3	2:A:497:PRO:HD3	1.87	0.56
2:B:620:MET:CG	2:B:664:LEU:HD12	2.35	0.56
1:D:8:DA:H4'	2:B:886:GLU:O	2.05	0.56
2:A:336:GLN:NE2	2:A:417:TYR:H	1.94	0.56
2:B:710:LYS:O	2:B:712:PRO:HD3	2.05	0.56
2:A:654:ILE:HD11	2:A:668:ILE:HG21	1.86	0.56
2:A:718:MET:HE2	2:A:728:GLU:HA	1.88	0.56
2:B:701:MET:O	2:B:704:VAL:HG12	2.05	0.56
2:B:620:MET:HG2	2:B:664:LEU:HD12	1.87	0.55
2:B:416:ALA:O	2:B:428:LEU:HD23	2.06	0.55
2:B:63:SER:OG	2:B:67:ARG:HD2	2.06	0.55
2:B:262:ILE:HD12	2:B:262:ILE:N	2.21	0.55
2:A:336:GLN:HE21	2:A:417:TYR:N	1.95	0.55
2:B:520:ASN:HD21	2:B:527:LYS:NZ	2.04	0.55
2:A:1094:GLU:HG2	2:A:1098:ARG:HD3	1.89	0.55
2:A:718:MET:CE	2:A:728:GLU:HA	2.36	0.55
1:C:11:DT:H5'	2:A:269:THR:O	2.07	0.55
2:A:512:PRO:HB2	2:A:514:ASN:ND2	2.22	0.55
2:A:714:ILE:CG2	2:A:719:ALA:HB2	2.34	0.55
2:A:263:ASP:O	2:A:265:ASP:N	2.40	0.54
2:A:830:MET:O	2:A:834:ARG:HG2	2.06	0.54
2:B:416:ALA:C	2:B:428:LEU:HD23	2.28	0.54
2:B:870:ALA:HB2	2:B:989:LYS:HD3	1.89	0.54
2:A:794:VAL:O	2:A:798:ARG:HG2	2.06	0.54
2:B:314:ASN:HB3	2:B:323:ARG:HH12	1.71	0.54
2:A:1014:TYR:HD1	2:A:1017:ARG:NH1	2.06	0.54
2:A:130:VAL:HA	2:A:133:LYS:HE3	1.90	0.54
2:B:173:LYS:HD2	2:B:197:PHE:O	2.06	0.54
2:B:715:SER:O	2:B:716:ALA:HB3	2.07	0.54
2:A:833:GLN:O	2:A:837:GLU:HG3	2.08	0.54
2:A:816:LEU:CD1	2:A:983:VAL:HG21	2.38	0.54
2:A:370:GLU:HB2	2:A:773:LYS:HZ3	1.71	0.54
2:B:382:GLY:O	2:B:385:ARG:HG3	2.07	0.54
2:A:996:PHE:CG	2:A:1025:ILE:HD11	2.43	0.53
2:B:16:TYR:O	2:B:35:LYS:HE2	2.08	0.53
2:B:234:ILE:HB	2:B:235:PRO:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:620:MET:HE1	2:A:664:LEU:HB2	1.91	0.53
2:A:467:LEU:O	2:A:471:LEU:HD22	2.08	0.53
2:A:764:THR:HG21	2:A:780:GLU:HB3	1.90	0.53
2:A:771:ASN:HD21	2:A:773:LYS:HB3	1.74	0.53
2:B:89:TYR:OH	2:B:284:ILE:HD11	2.08	0.53
2:B:37:SER:HB3	2:B:231:THR:HG22	1.91	0.53
2:B:816:LEU:HD11	2:B:983:VAL:HG21	1.91	0.53
2:A:783:LYS:O	2:A:787:GLU:HG2	2.09	0.53
2:B:694:THR:HG22	2:B:777:ILE:HD12	1.90	0.52
2:A:257:VAL:HG22	2:A:270:ILE:O	2.09	0.52
2:A:266:ASN:HD22	2:A:266:ASN:C	2.12	0.52
2:A:1045:ILE:HG23	2:A:1094:GLU:OE1	2.09	0.52
2:B:597:LYS:HZ3	2:B:602:HIS:HD2	1.56	0.52
2:A:1055:LEU:HD23	2:A:1069:ASN:ND2	2.25	0.52
2:A:82:ASN:ND2	2:A:85:VAL:H	2.07	0.52
2:B:1092:ARG:HG2	2:B:1092:ARG:HH11	1.75	0.52
1:C:5:DC:H5'	2:A:921:PRO:HG2	1.92	0.52
2:A:82:ASN:C	2:A:82:ASN:ND2	2.63	0.52
2:B:514:ASN:H	2:B:514:ASN:HD22	1.57	0.52
2:A:370:GLU:HA	2:A:773:LYS:NZ	2.25	0.52
2:A:958:ASN:HD22	2:A:958:ASN:N	2.02	0.52
2:B:1098:ARG:HG3	2:B:1098:ARG:O	2.10	0.52
2:A:289:THR:O	2:A:293:GLU:HG3	2.10	0.51
2:A:616:THR:HG22	2:A:620:MET:HE2	1.91	0.51
2:B:770:ILE:HG23	2:B:775:TYR:CD1	2.45	0.51
2:A:72:THR:O	2:A:74:LYS:HG3	2.10	0.51
2:B:82:ASN:C	2:B:82:ASN:HD22	2.14	0.51
2:B:336:GLN:NE2	2:B:417:TYR:H	1.97	0.51
1:C:4:DT:O4	2:A:688:LYS:HD2	2.11	0.51
2:A:1099:LYS:HG2	2:A:1100:GLN:N	2.24	0.51
2:A:1053:VAL:O	2:A:1055:LEU:HD22	2.11	0.51
2:A:267:LYS:H	2:A:267:LYS:CD	2.20	0.51
2:A:369:LYS:HA	2:A:372:LEU:HD21	1.93	0.51
2:A:372:LEU:HD12	2:A:380:LEU:HD12	1.91	0.51
2:B:1099:LYS:HB3	2:B:1100:GLN:OE1	2.10	0.51
2:A:791:HIS:HA	2:A:795:GLU:HG3	1.92	0.51
2:B:578:THR:HG23	2:B:579:PRO:HD2	1.93	0.51
2:A:752:LYS:HZ3	2:A:755:GLY:HA2	1.75	0.50
2:A:958:ASN:H	2:A:958:ASN:ND2	2.03	0.50
2:B:704:VAL:HG23	2:B:719:ALA:HB1	1.93	0.50
2:B:355:LYS:HD2	2:B:388:GLU:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:514:ASN:HD22	2:A:514:ASN:H	1.57	0.50
2:A:708:ARG:HG2	2:A:714:ILE:HG22	1.93	0.50
2:B:213:LYS:HE3	2:B:292:GLU:OE2	2.11	0.50
2:B:578:THR:CG2	2:B:579:PRO:HD2	2.42	0.50
2:B:673:LEU:O	2:B:677:ILE:HD13	2.10	0.50
2:A:454:ASN:HD22	2:A:457:ASN:HD21	1.58	0.50
2:A:671:ASN:C	2:A:671:ASN:HD22	2.15	0.50
2:B:8:LEU:HD23	2:B:39:THR:HG21	1.93	0.50
2:B:1088:ASN:O	2:B:1092:ARG:HG3	2.11	0.50
2:A:355:LYS:HD2	2:A:388:GLU:HG3	1.93	0.50
2:B:369:LYS:HE3	2:B:377:ALA:HB1	1.93	0.50
2:A:1005:GLU:HG2	2:A:1009:LYS:HE3	1.91	0.50
2:B:968:ASN:HD21	2:B:1060:MET:H	1.59	0.50
2:A:587:LYS:NZ	2:A:607:ASP:OD2	2.45	0.50
2:A:639:GLN:HE22	2:A:744:THR:HB	1.77	0.50
2:B:1061:ALA:O	2:B:1062:ALA:HB2	2.12	0.50
2:B:918:ALA:C	2:B:921:PRO:HD2	2.33	0.50
2:A:89:TYR:O	2:A:93:MET:HG2	2.12	0.49
2:B:176:LYS:C	2:B:176:LYS:HD3	2.32	0.49
2:A:127:ASN:H	2:A:127:ASN:ND2	2.01	0.49
2:B:393:GLN:HG2	2:B:431:TYR:HB2	1.94	0.49
2:A:565:PRO:HA	2:A:677:ILE:HG12	1.95	0.49
2:B:649:LEU:HB3	2:B:650:PHE:CD1	2.48	0.49
2:B:65:ARG:O	2:B:69:GLU:HG3	2.13	0.49
2:B:347:VAL:O	2:B:351:GLU:HG3	2.13	0.49
2:A:306:GLY:O	2:A:414:HIS:HE1	1.96	0.49
2:A:1014:TYR:HA	2:A:1017:ARG:CZ	2.43	0.49
2:B:24:ASP:HB3	2:B:27:ALA:CB	2.32	0.49
2:B:198:ASP:OD2	2:B:385:ARG:NH2	2.40	0.49
2:A:257:VAL:HG23	2:A:257:VAL:O	2.12	0.49
2:A:12:ILE:HA	2:A:40:LEU:HD11	1.95	0.49
2:B:196:GLN:O	2:B:199:THR:HG22	2.13	0.49
2:A:370:GLU:HB2	2:A:773:LYS:NZ	2.28	0.49
2:A:1099:LYS:CG	2:A:1100:GLN:H	2.26	0.49
2:A:176:LYS:HD3	2:A:177:ASP:N	2.27	0.49
2:A:918:ALA:C	2:A:921:PRO:HD2	2.32	0.49
2:A:1012:LEU:HD11	2:A:1025:ILE:HG22	1.95	0.48
2:B:364:ALA:N	2:B:384:ASN:HD21	2.02	0.48
2:A:980:ILE:HG23	2:A:1036:LEU:HD12	1.94	0.48
2:B:868:ASN:OD1	2:B:869:LEU:HD22	2.13	0.48
2:B:319:ASN:HD22	2:B:319:ASN:HA	1.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:675:ILE:HD11	2:B:685:ILE:HG12	1.94	0.48
1:C:7:DA:C4	2:A:318:ARG:HD3	2.48	0.48
2:B:135:LEU:O	2:B:138:VAL:HG22	2.13	0.48
2:A:373:ASN:HD22	2:A:376:HIS:H	1.61	0.48
2:A:1096:GLU:O	2:A:1099:LYS:HB3	2.14	0.48
2:A:118:LYS:O	2:A:122:GLN:HG3	2.14	0.48
2:A:438:LEU:HD12	2:A:529:PHE:CZ	2.48	0.48
2:A:968:ASN:ND2	2:A:1060:MET:H	2.10	0.48
2:A:620:MET:HG3	2:A:664:LEU:HD12	1.96	0.48
2:B:249:SER:O	2:B:250:THR:CG2	2.60	0.48
2:B:18:SER:HB2	2:B:139:GLU:OE2	2.13	0.48
2:B:182:THR:HA	2:B:270:ILE:CD1	2.43	0.48
2:B:619:LEU:HD22	2:B:797:LEU:HD13	1.96	0.48
2:A:809:LEU:O	2:A:813:THR:HG23	2.14	0.48
2:A:834:ARG:HG3	2:A:834:ARG:HH11	1.77	0.48
2:B:317:LEU:HG	2:B:318:ARG:HH11	1.77	0.48
2:B:446:THR:O	2:B:447:LYS:HG3	2.14	0.48
2:B:857:LYS:HE2	2:B:861:ASP:OD2	2.13	0.48
1:D:6:DA:H3'	1:D:7:DA:H5"	1.95	0.48
2:A:197:PHE:HZ	2:A:257:VAL:HG21	1.77	0.48
2:A:358:ILE:HD12	2:A:391:TYR:CE1	2.49	0.48
2:B:336:GLN:HE21	2:B:417:TYR:N	1.98	0.48
2:A:336:GLN:O	2:A:414:HIS:HD2	1.96	0.47
2:A:795:GLU:HB2	2:A:796:PRO:CD	2.45	0.47
2:B:597:LYS:HE2	2:B:602:HIS:HB2	1.96	0.47
2:A:443:ILE:C	2:A:444:LEU:HD22	2.34	0.47
2:A:725:ALA:HB2	2:A:734:LEU:HD12	1.97	0.47
2:A:891:ALA:HB2	2:A:909:ILE:CD1	2.45	0.47
2:A:752:LYS:HZ2	2:A:755:GLY:HA2	1.77	0.47
2:A:1057:ILE:N	2:A:1057:ILE:HD12	2.29	0.47
2:A:197:PHE:CZ	2:A:257:VAL:HG21	2.50	0.47
2:B:51:SER:O	2:B:150:GLN:HG3	2.14	0.47
2:B:665:LYS:O	2:B:668:ILE:HG13	2.14	0.47
2:A:263:ASP:O	2:A:263:ASP:CG	2.53	0.47
2:A:1017:ARG:HG2	2:A:1017:ARG:HH11	1.80	0.47
2:B:802:THR:HG23	2:B:810:VAL:HG21	1.97	0.47
2:B:592:ILE:HG12	2:B:1055:LEU:CD2	2.45	0.47
2:A:1061:ALA:O	2:A:1062:ALA:CB	2.62	0.47
2:A:304:PHE:HB3	2:A:308:ASP:O	2.14	0.46
2:B:1053:VAL:HG12	2:B:1054:ASN:N	2.30	0.46
2:A:514:ASN:HD22	2:A:514:ASN:N	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:ARG:HD2	2:B:294:ALA:O	2.16	0.46
1:D:6:DA:H3'	1:D:7:DA:C5'	2.44	0.46
2:A:207:VAL:HG11	2:A:905:VAL:HG21	1.98	0.46
2:A:318:ARG:CB	2:A:421:ARG:HH12	2.26	0.46
2:A:603:ARG:HH11	2:A:603:ARG:HB3	1.80	0.46
2:B:704:VAL:HG23	2:B:719:ALA:CB	2.45	0.46
2:B:715:SER:HB3	2:B:718:MET:CB	2.43	0.46
2:A:490:LEU:HG	2:A:495:LEU:HG	1.97	0.46
2:A:730:HIS:O	2:A:733:GLU:HG2	2.15	0.46
2:B:704:VAL:O	2:B:708:ARG:HG2	2.15	0.46
2:A:258:ASP:OD2	2:A:261:GLU:HG2	2.14	0.46
2:A:1099:LYS:CG	2:A:1100:GLN:N	2.78	0.46
2:B:662:LEU:HD22	2:B:664:LEU:HG	1.98	0.46
2:B:1086:GLU:OE2	2:B:1089:LYS:HE3	2.15	0.46
2:B:639:GLN:NE2	2:B:744:THR:CG2	2.79	0.46
2:B:704:VAL:HG11	2:B:772:PRO:HB3	1.97	0.46
2:B:15:VAL:HG21	2:B:40:LEU:HD21	1.98	0.46
2:B:41:PRO:HB3	2:B:45:LYS:HE2	1.97	0.46
2:B:316:GLN:NE2	2:B:421:ARG:HA	2.31	0.46
2:A:373:ASN:ND2	2:A:375:ASN:H	2.12	0.46
2:A:404:GLN:O	2:A:405:SER:HB3	2.15	0.46
2:A:1061:ALA:O	2:A:1062:ALA:HB2	2.15	0.46
2:A:317:LEU:HD11	2:A:318:ARG:HH21	1.80	0.45
2:A:864:ALA:O	2:A:867:ASN:ND2	2.50	0.45
2:A:1100:GLN:O	2:A:1101:LYS:CG	2.63	0.45
2:B:20:VAL:HG23	2:B:138:VAL:O	2.16	0.45
2:B:514:ASN:HD22	2:B:514:ASN:N	2.12	0.45
2:A:88:ARG:HB3	2:A:284:ILE:HG13	1.97	0.45
2:A:444:LEU:HD22	2:A:444:LEU:N	2.31	0.45
2:A:444:LEU:N	2:A:444:LEU:CD2	2.80	0.45
2:A:1045:ILE:HD13	2:A:1098:ARG:NH1	2.31	0.45
2:B:1045:ILE:HG23	2:B:1094:GLU:CG	2.42	0.45
2:A:725:ALA:HB2	2:A:734:LEU:CD1	2.46	0.45
2:B:764:THR:HG22	2:B:764:THR:O	2.17	0.45
2:A:243:LEU:O	2:A:247:VAL:HG23	2.16	0.45
2:A:815:GLN:HE21	2:A:1035:ASN:HB2	1.82	0.45
2:B:1016:GLN:O	2:B:1020:ALA:HB2	2.16	0.45
2:A:343:HIS:HE1	2:A:537:GLU:OE2	2.00	0.45
2:B:197:PHE:CD1	2:B:272:LEU:HD21	2.51	0.45
2:B:668:ILE:HD12	2:B:669:ALA:N	2.31	0.45
2:A:65:ARG:O	2:A:69:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:158:ALA:CA	2:A:213:LYS:HZ2	2.28	0.45
2:A:454:ASN:HB3	2:A:457:ASN:ND2	2.32	0.45
2:A:740:LYS:HD2	2:A:740:LYS:C	2.37	0.45
2:B:344:THR:HB	2:B:345:PRO:HD3	1.97	0.45
2:B:932:MET:HE2	2:B:1060:MET:SD	2.57	0.45
2:B:1045:ILE:HD12	2:B:1094:GLU:HG3	1.97	0.45
2:A:210:LEU:HB3	2:A:239:ALA:HB1	1.97	0.45
2:A:234:ILE:HB	2:A:235:PRO:HD3	1.97	0.45
2:B:560:GLY:HA2	2:B:1059:GLN:O	2.16	0.45
2:A:161:GLN:HB3	2:A:213:LYS:HZ2	1.74	0.45
2:B:304:PHE:CG	2:B:310:PRO:HG3	2.52	0.45
2:B:343:HIS:CD2	2:B:345:PRO:HD2	2.52	0.45
2:A:263:ASP:HA	2:A:264:PRO:HD2	1.63	0.45
2:B:593:GLY:HA2	2:B:1054:ASN:HD21	1.80	0.45
2:A:771:ASN:ND2	2:A:773:LYS:HB3	2.32	0.44
2:A:512:PRO:HB2	2:A:514:ASN:HD22	1.80	0.44
2:A:1041:LEU:C	2:A:1041:LEU:HD13	2.37	0.44
2:A:319:ASN:N	2:A:320:PRO:HD3	2.32	0.44
2:A:397:VAL:O	2:A:401:VAL:HG23	2.17	0.44
2:A:864:ALA:HA	2:A:867:ASN:HD21	1.83	0.44
2:B:909:ILE:C	2:B:909:ILE:HD12	2.38	0.44
2:A:66:ALA:O	2:A:70:LEU:HD22	2.18	0.44
2:A:176:LYS:HD3	2:A:176:LYS:C	2.38	0.44
2:A:649:LEU:HD13	2:A:737:ARG:NH2	2.32	0.44
2:B:562:THR:HG22	2:B:612:TYR:CZ	2.51	0.44
2:A:267:LYS:HD3	2:A:267:LYS:N	2.31	0.44
2:B:650:PHE:HE2	2:B:700:ARG:HG3	1.82	0.44
2:B:655:ASN:HD22	2:B:655:ASN:N	2.14	0.44
2:A:158:ALA:CA	2:A:213:LYS:NZ	2.68	0.44
2:A:802:THR:HG23	2:A:810:VAL:HG21	1.99	0.44
2:A:822:ILE:CD1	2:A:1032:ILE:HD12	2.47	0.44
2:A:671:ASN:ND2	2:A:675:ILE:HG23	2.33	0.44
2:A:805:VAL:HB	2:A:809:LEU:HD23	2.00	0.44
2:B:577:PHE:HE2	2:B:1050:LEU:HD21	1.83	0.44
2:A:13:ASP:O	2:A:17:PRO:HG3	2.17	0.44
2:A:88:ARG:HG3	2:A:283:PRO:HB2	1.99	0.44
2:A:673:LEU:O	2:A:677:ILE:HD13	2.18	0.44
2:A:1004:LEU:O	2:A:1004:LEU:HD13	2.18	0.44
1:D:7:DA:C5	2:B:318:ARG:NE	2.85	0.43
2:A:306:GLY:O	2:A:414:HIS:CE1	2.71	0.43
2:A:323:ARG:HD2	3:A:1298:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:771:ASN:C	2:A:773:LYS:H	2.22	0.43
2:B:829:ASP:O	2:B:833:GLN:HG3	2.18	0.43
2:B:595:PRO:O	2:B:596:ASN:HB2	2.18	0.43
2:B:520:ASN:HD21	2:B:527:LYS:HZ2	1.66	0.43
2:B:598:THR:OG1	2:B:601:GLU:HG3	2.18	0.43
2:B:995:ASP:OD2	2:B:998:LYS:HG2	2.16	0.43
2:B:303:MET:CE	2:B:400:GLN:NE2	2.82	0.43
2:B:700:ARG:NH2	2:B:723:LYS:CD	2.70	0.43
2:A:127:ASN:N	2:A:127:ASN:ND2	2.63	0.43
2:A:454:ASN:ND2	2:A:457:ASN:ND2	2.66	0.43
2:A:815:GLN:HE21	2:A:1035:ASN:CB	2.31	0.43
2:A:1014:TYR:HA	2:A:1017:ARG:CD	2.47	0.43
2:B:831:PHE:HD2	2:B:866:LEU:HD11	1.82	0.43
2:A:1005:GLU:CG	2:A:1009:LYS:HE3	2.48	0.43
2:A:771:ASN:C	2:A:771:ASN:HD22	2.21	0.43
2:A:849:LYS:HG2	2:A:850:LYS:N	2.34	0.43
2:A:1053:VAL:O	2:A:1055:LEU:CD2	2.67	0.43
2:B:766:ALA:O	2:B:767:LYS:O	2.37	0.43
2:A:597:LYS:HZ3	2:A:602:HIS:HD2	1.64	0.43
2:B:446:THR:C	2:B:447:LYS:HG3	2.39	0.43
2:A:570:MET:HG2	2:A:585:ILE:HD11	2.01	0.43
2:A:101:ASP:OD1	2:B:109:LYS:HE3	2.18	0.42
2:A:372:LEU:N	2:A:372:LEU:HD23	2.33	0.42
2:A:1041:LEU:O	2:A:1045:ILE:HG12	2.19	0.42
2:B:28:GLU:CD	2:B:29:GLY:N	2.72	0.42
2:B:855:THR:OG1	2:B:858:GLU:HG3	2.19	0.42
2:A:995:ASP:OD1	2:A:998:LYS:HD2	2.19	0.42
2:A:1025:ILE:C	2:A:1025:ILE:HD12	2.39	0.42
2:A:1072:LYS:HA	2:A:1072:LYS:HD3	1.70	0.42
2:B:740:LYS:HE2	2:B:740:LYS:HB3	1.88	0.42
2:B:890:VAL:HG21	2:B:909:ILE:HD11	2.01	0.42
2:A:343:HIS:CD2	2:A:345:PRO:HD2	2.54	0.42
2:A:864:ALA:HA	2:A:867:ASN:ND2	2.34	0.42
2:A:633:ASN:OD1	2:A:635:PRO:HD2	2.20	0.42
2:B:1018:GLU:OE1	2:B:1018:GLU:N	2.51	0.42
1:C:5:DC:H2"	1:C:6:DA:O5'	2.19	0.42
1:D:7:DA:H2"	1:D:8:DA:OP2	2.19	0.42
2:A:683:ARG:HG3	2:A:683:ARG:HH11	1.83	0.42
2:B:178:VAL:HG21	2:B:194:VAL:HG13	2.01	0.42
2:B:406:GLU:HG3	2:B:407:ASP:N	2.33	0.42
2:B:717:ALA:HA	2:B:735:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:771:ASN:O	2:B:775:TYR:N	2.47	0.42
2:B:868:ASN:ND2	2:B:993:ASN:HB3	2.35	0.42
2:B:1048:LYS:HE2	2:B:1048:LYS:HB3	1.83	0.42
2:A:653:ASP:HB2	2:A:668:ILE:HG23	2.01	0.42
2:B:314:ASN:HB3	2:B:323:ARG:NH1	2.35	0.42
2:A:135:LEU:O	2:A:138:VAL:HG22	2.19	0.42
2:B:969:GLU:O	2:B:973:THR:HG23	2.20	0.42
2:A:633:ASN:CG	2:A:636:ILE:HG12	2.39	0.42
2:A:717:ALA:HB1	2:A:732:GLU:HA	2.02	0.42
2:A:1013:GLU:OE1	2:A:1013:GLU:HA	2.20	0.42
2:B:766:ALA:HA	2:B:781:GLN:NE2	2.35	0.42
2:A:650:PHE:HB3	2:A:696:ALA:CB	2.50	0.42
2:A:651:LEU:HA	2:A:652:PRO:HD3	1.85	0.42
2:A:891:ALA:HB2	2:A:909:ILE:HD12	2.00	0.42
2:B:279:ASP:HB3	2:B:281:PHE:CE1	2.55	0.42
2:B:351:GLU:HG2	2:B:395:PHE:CE2	2.55	0.42
2:B:597:LYS:HZ1	2:B:602:HIS:HD2	1.66	0.42
2:B:769:LYS:HD2	2:B:769:LYS:HA	1.92	0.42
2:A:360:GLU:HA	2:A:365:GLY:CA	2.50	0.41
2:A:678:TYR:O	2:A:921:PRO:HG3	2.20	0.41
2:B:303:MET:HE3	2:B:400:GLN:NE2	2.35	0.41
2:B:438:LEU:C	2:B:438:LEU:HD23	2.40	0.41
2:B:639:GLN:NE2	2:B:744:THR:HG22	2.35	0.41
2:A:650:PHE:HE2	2:A:700:ARG:HG3	1.84	0.41
2:A:1032:ILE:HG22	2:A:1036:LEU:HD23	2.03	0.41
2:B:570:MET:HG2	2:B:975:TRP:CG	2.55	0.41
1:C:15:DG:N7	2:A:114:LYS:NZ	2.58	0.41
2:A:144:THR:HB	2:A:145:PHE:H	1.66	0.41
2:A:304:PHE:CD2	2:A:310:PRO:HG3	2.55	0.41
2:A:629:ASN:N	2:A:629:ASN:HD22	2.18	0.41
2:B:16:TYR:O	2:B:35:LYS:CE	2.69	0.41
2:B:257:VAL:HG12	2:B:259:MET:CE	2.50	0.41
2:A:360:GLU:HA	2:A:365:GLY:HA2	2.03	0.41
2:B:319:ASN:N	2:B:320:PRO:HD3	2.36	0.41
2:B:1098:ARG:O	2:B:1098:ARG:CG	2.68	0.41
2:A:639:GLN:NE2	2:A:744:THR:HB	2.35	0.41
2:A:714:ILE:CD1	2:A:718:MET:HB3	2.51	0.41
2:A:771:ASN:ND2	2:A:771:ASN:C	2.74	0.41
2:A:791:HIS:HA	2:A:795:GLU:CG	2.51	0.41
2:B:130:VAL:HA	2:B:133:LYS:HE3	2.03	0.41
2:A:69:GLU:HB3	2:A:74:LYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:258:ASP:OD2	2:A:260:SER:OG	2.37	0.41
2:A:383:LYS:HE3	2:A:383:LYS:HB2	1.91	0.41
2:A:1075:LEU:HA	2:A:1078:MET:CE	2.50	0.41
2:B:258:ASP:OD1	2:B:260:SER:OG	2.38	0.41
2:B:440:ARG:O	2:B:444:LEU:HD13	2.21	0.41
2:A:266:ASN:ND2	2:A:266:ASN:C	2.74	0.41
2:A:816:LEU:HD13	2:A:983:VAL:HG21	2.03	0.41
2:B:481:GLU:H	2:B:481:GLU:CD	2.23	0.41
2:A:189:LEU:HD22	2:A:193:LEU:HD23	2.03	0.41
2:A:384:ASN:HD22	2:A:384:ASN:HA	1.65	0.41
2:A:886:GLU:HG2	2:A:908:SER:HB3	2.03	0.41
2:A:958:ASN:N	2:A:958:ASN:ND2	2.66	0.41
2:A:1032:ILE:O	2:A:1036:LEU:CD2	2.67	0.41
2:B:84:GLU:O	2:B:88:ARG:HG2	2.21	0.41
2:B:144:THR:CG2	2:B:145:PHE:H	2.00	0.41
2:B:633:ASN:OD1	2:B:635:PRO:HD2	2.20	0.41
2:B:662:LEU:HD23	2:B:663:GLU:N	2.36	0.41
2:B:936:LEU:HD13	2:B:967:ALA:HA	2.03	0.41
2:B:1061:ALA:O	2:B:1062:ALA:CB	2.68	0.41
2:A:256:ILE:HD13	2:A:271:GLY:HA2	2.02	0.41
2:A:853:PHE:CE2	2:A:909:ILE:HD13	2.55	0.41
2:A:967:ALA:HB1	2:A:1060:MET:HG3	2.02	0.41
2:B:185:ASP:OD2	2:B:187:ALA:HB3	2.21	0.41
2:B:650:PHE:HB3	2:B:696:ALA:CB	2.51	0.41
2:B:651:LEU:HA	2:B:652:PRO:HD3	1.76	0.41
2:B:16:TYR:OH	2:B:150:GLN:NE2	2.54	0.40
2:B:309:ILE:HA	2:B:310:PRO:HD3	1.95	0.40
2:B:367:LEU:HD21	2:B:380:LEU:HB3	2.02	0.40
2:B:620:MET:HG3	2:B:664:LEU:HD12	2.03	0.40
2:A:1017:ARG:NH1	2:A:1017:ARG:HG2	2.37	0.40
2:B:181:ILE:HD13	2:B:202:THR:HG21	2.03	0.40
2:B:561:VAL:O	2:B:562:THR:C	2.59	0.40
2:B:612:TYR:CZ	2:B:670:LYS:CD	3.04	0.40
2:B:649:LEU:HD13	2:B:737:ARG:CZ	2.50	0.40
2:A:432:ASN:HB2	2:A:433:PRO:CD	2.51	0.40
2:A:831:PHE:O	2:A:835:VAL:HG23	2.21	0.40
2:A:182:THR:HG21	2:A:193:LEU:HD21	2.03	0.40
2:A:711:ASP:OD1	2:A:713:ASN:HB2	2.22	0.40
2:B:566:ILE:HG13	2:B:588:GLY:HA3	2.03	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	1091/1117 (98%)	1048 (96%)	34 (3%)	9 (1%)	19	13
2	B	1091/1117 (98%)	1050 (96%)	33 (3%)	8 (1%)	22	16
All	All	2182/2234 (98%)	2098 (96%)	67 (3%)	17 (1%)	19	13

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	264	PRO
2	A	369	LYS
2	A	1014	TYR
2	A	1062	ALA
2	A	1101	LYS
2	B	724	GLN
2	B	726	ALA
2	B	767	LYS
2	B	850	LYS
2	B	1062	ALA
2	B	723	LYS
2	B	727	SER
2	B	851	GLY
2	A	370	GLU
2	A	670	LYS
2	A	1099	LYS
2	A	772	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	913/934 (98%)	880 (96%)	33 (4%)	35	34
2	B	914/934 (98%)	884 (97%)	30 (3%)	38	37
All	All	1827/1868 (98%)	1764 (97%)	63 (3%)	37	36

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	70	LEU
2	A	82	ASN
2	A	88	ARG
2	A	127	ASN
2	A	163	ARG
2	A	191	GLU
2	A	210	LEU
2	A	212	GLN
2	A	266	ASN
2	A	267	LYS
2	A	292	GLU
2	A	309	ILE
2	A	318	ARG
2	A	319	ASN
2	A	368	ASN
2	A	385	ARG
2	A	444	LEU
2	A	471	LEU
2	A	472	ASP
2	A	483	MET
2	A	484	SER
2	A	514	ASN
2	A	603	ARG
2	A	623	LEU
2	A	648	ASP
2	A	671	ASN
2	A	714	ILE
2	A	771	ASN
2	A	817	GLN
2	A	838	LYS
2	A	958	ASN
2	A	1017	ARG
2	A	1096	GLU
2	B	28	GLU

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Mol	Chain	Res	Type
2	B	52	GLU
2	B	70	LEU
2	B	82	ASN
2	B	127	ASN
2	B	163	ARG
2	B	250	THR
2	B	281	PHE
2	B	284	ILE
2	B	319	ASN
2	B	368	ASN
2	B	406	GLU
2	B	444	LEU
2	B	471	LEU
2	B	483	MET
2	B	514	ASN
2	B	520	ASN
2	B	541	TYR
2	B	580	ASP
2	B	603	ARG
2	B	623	LEU
2	B	662	LEU
2	B	670	LYS
2	B	771	ASN
2	B	795	GLU
2	B	817	GLN
2	B	838	LYS
2	B	886	GLU
2	B	1041	LEU
2	B	1050	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	82	ASN
2	A	127	ASN
2	A	150	GLN
2	A	169	ASN
2	A	186	GLN
2	A	212	GLN
2	A	266	ASN
2	A	298	ASN
2	A	316	GLN

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Mol	Chain	Res	Type
2	A	319	ASN
2	A	324	ASN
2	A	336	GLN
2	A	343	HIS
2	A	348	GLN
2	A	373	ASN
2	A	375	ASN
2	A	384	ASN
2	A	414	HIS
2	A	455	GLN
2	A	457	ASN
2	A	469	GLN
2	A	494	ASN
2	A	506	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	791	HIS
2	A	815	GLN
2	A	817	GLN
2	A	823	GLN
2	A	863	GLN
2	A	867	ASN
2	A	954	ASN
2	A	958	ASN
2	A	968	ASN
2	A	982	ASN
2	A	1035	ASN
2	A	1038	ASN
2	A	1047	HIS
2	A	1059	GLN
2	B	82	ASN
2	B	127	ASN
2	B	150	GLN
2	B	186	GLN
2	B	255	ASN
2	B	314	ASN

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Mol	Chain	Res	Type
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	375	ASN
2	B	376	HIS
2	B	384	ASN
2	B	414	HIS
2	B	457	ASN
2	B	469	GLN
2	B	494	ASN
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	730	HIS
2	B	771	ASN
2	B	781	GLN
2	B	786	GLN
2	B	815	GLN
2	B	817	GLN
2	B	833	GLN
2	B	892	ASN
2	B	914	GLN
2	B	954	ASN
2	B	958	ASN
2	B	968	ASN
2	B	1019	ASN
2	B	1035	ASN
2	B	1047	HIS
2	B	1059	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	20/33 (60%)	0.07	1 (5%) 28 28	22, 42, 66, 71	0
1	D	19/33 (57%)	-0.09	0 100 100	21, 33, 52, 54	0
2	A	1093/1117 (97%)	0.12	44 (4%) 38 37	9, 25, 53, 76	0
2	B	1093/1117 (97%)	0.11	39 (3%) 42 42	9, 23, 53, 83	0
All	All	2225/2300 (96%)	0.11	84 (3%) 40 39	9, 24, 53, 83	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	1102	VAL	10.1
2	A	1014	TYR	8.8
2	B	725	ALA	8.6
2	B	1099	LYS	7.3
2	B	724	GLN	6.5
2	B	723	LYS	5.4
2	B	8	LEU	5.4
2	B	1100	GLN	5.3
2	B	726	ALA	5.2
2	A	1103	ALA	5.1
2	A	726	ALA	4.8
2	B	712	PRO	4.6
2	A	723	LYS	4.5
2	A	1100	GLN	4.2
2	B	1014	TYR	4.1
2	A	1018	GLU	4.0
2	A	727	SER	3.8
2	B	264	PRO	3.8
2	A	1019	ASN	3.7
2	B	713	ASN	3.7
2	B	769	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
2	A	1015	ASP	3.6
2	B	768	GLY	3.6
2	B	727	SER	3.6
2	A	725	ALA	3.5
2	B	708	ARG	3.4
2	A	710	LYS	3.4
2	B	265	ASP	3.4
2	B	704	VAL	3.4
2	B	766	ALA	3.3
2	B	729	ALA	3.3
2	A	262	ILE	3.2
2	B	715	SER	3.1
2	A	1101	LYS	3.1
2	B	764	THR	3.1
2	A	730	HIS	3.1
2	B	754	LYS	3.1
2	A	724	GLN	3.1
2	B	1018	GLU	3.1
2	A	729	ALA	3.0
2	B	770	ILE	3.0
2	B	730	HIS	3.0
1	C	3	DG	3.0
2	A	264	PRO	2.9
2	B	1019	ASN	2.9
2	A	754	LYS	2.8
2	A	766	ALA	2.8
2	B	714	ILE	2.8
2	A	714	ILE	2.8
2	A	366	THR	2.7
2	B	1095	LEU	2.7
2	B	10	GLU	2.7
2	A	371	LEU	2.6
2	A	1013	GLU	2.6
2	B	1096	GLU	2.6
2	A	767	LYS	2.5
2	B	767	LYS	2.5
2	A	28	GLU	2.5
2	A	43	GLU	2.5
2	A	42	GLU	2.4
2	B	1098	ARG	2.4
2	A	1094	GLU	2.4
2	A	1099	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	720	MET	2.3
2	A	1098	ARG	2.3
2	A	713	ASN	2.3
2	B	765	GLY	2.3
2	A	14	ALA	2.3
2	A	263	ASP	2.3
2	A	719	ALA	2.2
2	B	260	SER	2.2
2	A	261	GLU	2.2
2	A	722	GLY	2.2
2	A	265	ASP	2.2
2	A	708	ARG	2.2
2	A	367	LEU	2.1
2	B	281	PHE	2.1
2	A	1096	GLU	2.1
2	A	756	VAL	2.1
2	A	709	ALA	2.1
2	B	42	GLU	2.1
2	B	774	THR	2.0
2	A	267	LYS	2.0
2	B	266	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 (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.