Full wwPDB X-ray Structure Validation Report ⓘ

Feb 11, 2024 – 10:17 AM EST

PDB ID	:	3C46
Title	:	X-ray crystal structure of the N4 mini-vRNAP P2_7a promoter complex soaked with MgCl2
Authors	:	Gleghorn, M.L.; Murakami, K.S.
Deposited on	:	2008-01-29
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:

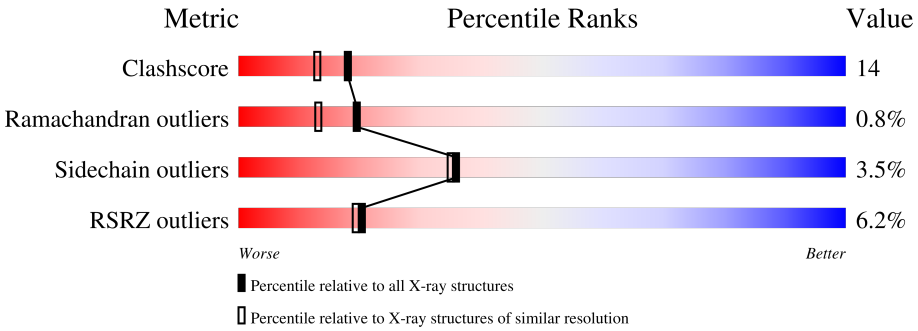
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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	A	1117	6%, 70%, 25%, • •
1	B	1117	6%, 75%, 21%, • •
2	C	36	6%, 39%, 17%, 44%
2	D	36	6%, 42%, 17%, 42%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18696 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 Virion RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1095	Total	C	N	O	S	0	0	0
			8454	5306	1435	1672	41			
1	B	1094	Total	C	N	O	S	0	0	0
			8443	5299	1432	1671	41			

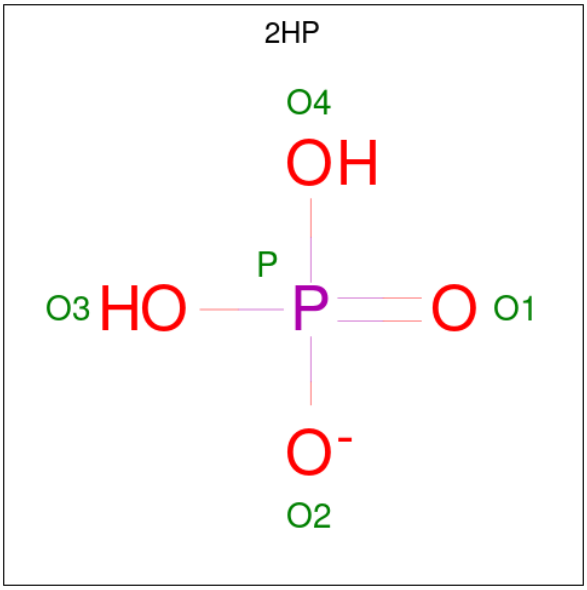
There are 24 discrepancies between the modelled and reference sequences:

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
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 2 is a DNA chain called P2_7a Promoter DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	20	Total 393	C 185	N 79	O 110	P 19	0	0	0
2	D	21	Total 429	C 205	N 83	O 121	P 20	0	0	0

- Molecule 3 is DIHYDROGENPHOSPHATE ION (three-letter code: 2HP) (formula: H_2O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	P 1	0	0
3	B	1	Total 5	O 4	P 1	0	0

- Molecule 4 is water.

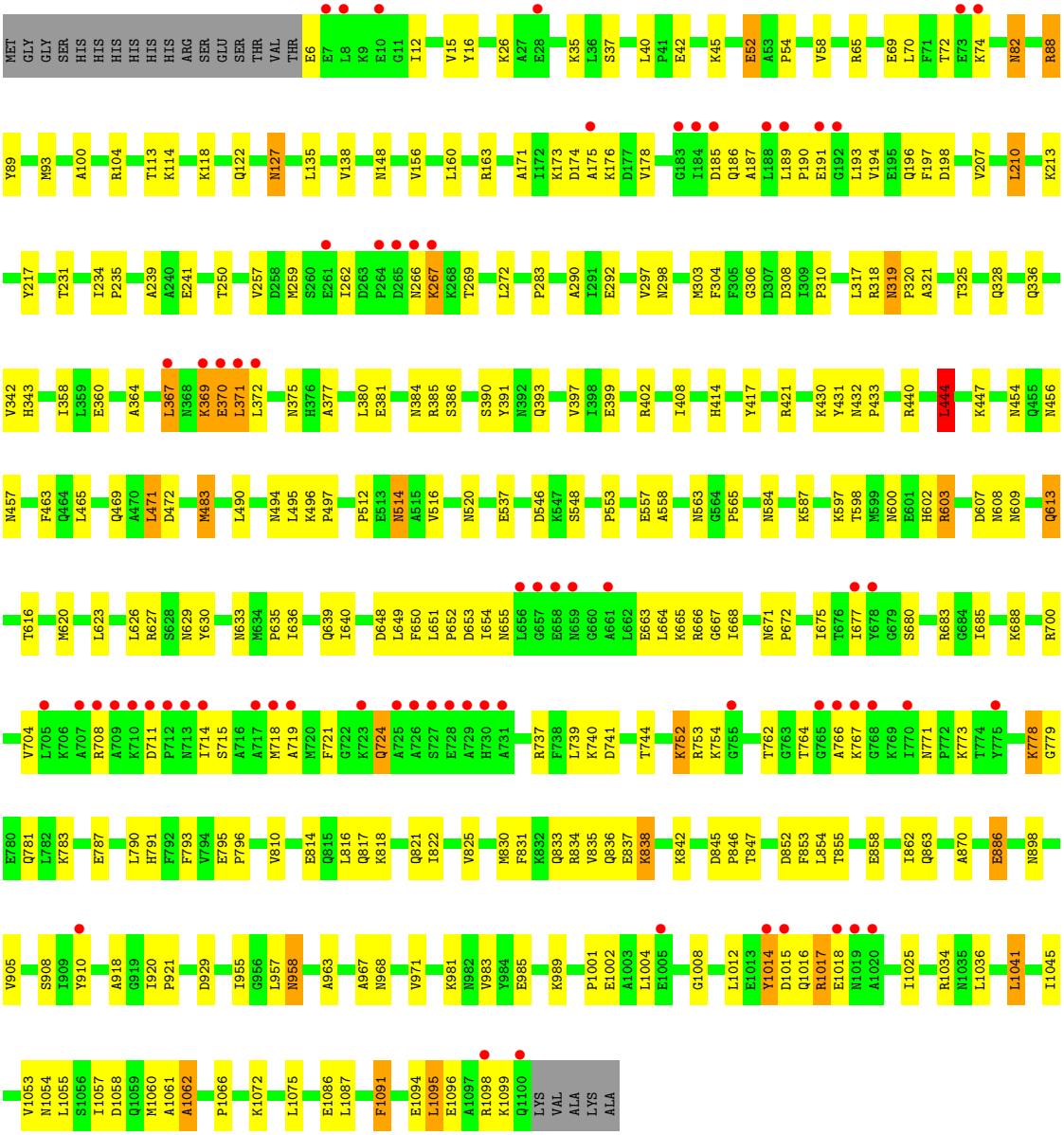
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	433	Total 433	O 433	0	0
4	C	27	Total 27	O 27	0	0
4	B	475	Total 475	O 475	0	0
4	D	32	Total 32	O 32	0	0

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.

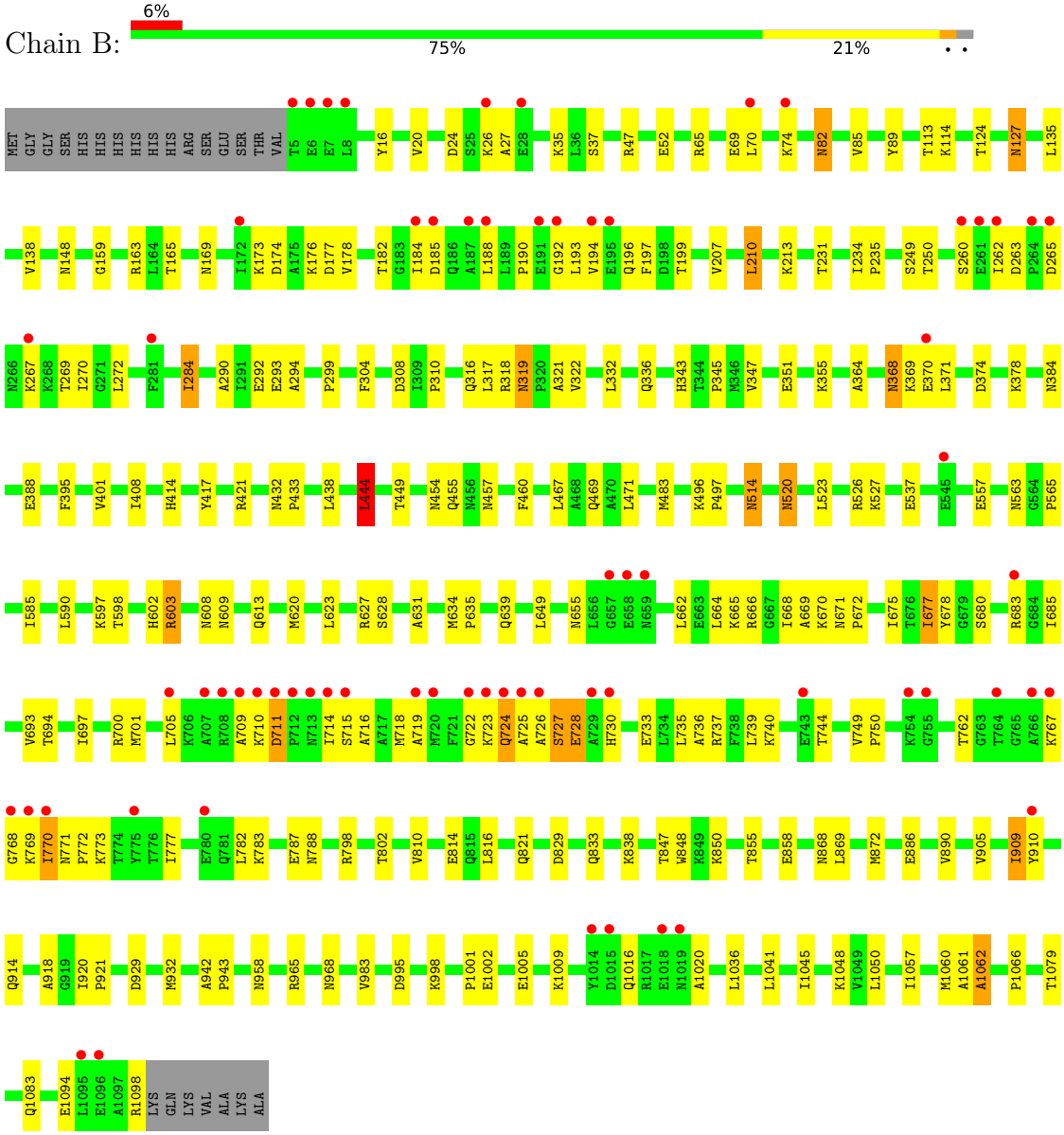
• Molecule 1: Virion RNA polymerase

Chain A:



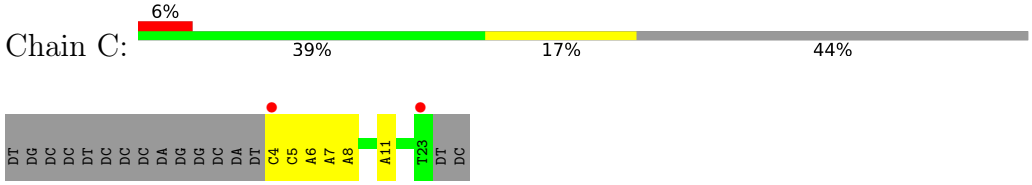
• Molecule 1: Virion RNA polymerase

Chain B:



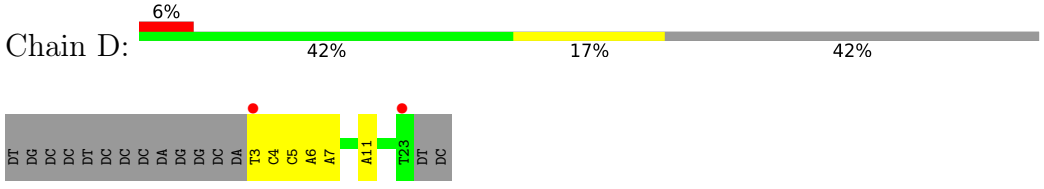
• Molecule 2: P2_7a Promoter DNA

Chain C:



• Molecule 2: P2_7a Promoter DNA

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.62Å 111.42Å 276.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 42.62 – 2.00	Depositor EDS
% Data completeness (in resolution range)	82.3 (50.00-2.00) 82.3 (42.62-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.242 0.207 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	20.2	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 45.3	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	18696	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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

Bond lengths and bond angles in the following residue types are not validated in this section: 2HP

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	0.33	0/8583	0.58	4/11609 (0.0%)
1	B	0.34	0/8572	0.58	2/11596 (0.0%)
2	C	0.29	0/442	0.69	0/681
2	D	0.33	0/482	0.72	0/742
All	All	0.33	0/18079	0.59	6/24628 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	444	LEU	CA-CB-CG	6.71	130.73	115.30
1	B	444	LEU	CA-CB-CG	5.85	128.75	115.30
1	A	852	ASP	N-CA-C	-5.62	95.81	111.00
1	A	558	ALA	N-CA-C	-5.38	96.48	111.00
1	B	148	ASN	N-CA-C	-5.21	96.93	111.00
1	A	148	ASN	N-CA-C	-5.05	97.35	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	A	8454	0	8479	264	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	8443	0	8465	206	0
2	C	393	0	212	10	0
2	D	429	0	237	10	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	433	0	0	3	0
4	B	475	0	0	3	0
4	C	27	0	0	1	0
4	D	32	0	0	1	0
All	All	18696	0	17393	474	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 (474) 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:680:SER:HA	2:D:4:DC:H5'	1.41	1.00
1:B:364:ALA:H	1:B:384:ASN:HD21	1.00	0.99
1:A:336:GLN:HE21	1:A:417:TYR:H	1.09	0.99
1:A:688:LYS:HD2	2:C:4:DC:H41	1.27	0.98
1:B:336:GLN:HE21	1:B:417:TYR:H	1.11	0.97
1:B:769:LYS:HG3	1:B:770:ILE:H	1.28	0.95
1:B:364:ALA:H	1:B:384:ASN:ND2	1.65	0.94
1:A:469:GLN:HE22	1:A:557:GLU:H	0.94	0.92
1:A:364:ALA:H	1:A:384:ASN:HD21	1.12	0.90
2:D:5:DC:H2"	2:D:6:DA:H5'	1.55	0.88
1:B:603:ARG:HH11	1:B:603:ARG:HB3	1.38	0.88
1:A:680:SER:HA	2:C:4:DC:H5'	1.55	0.87
1:B:469:GLN:HE22	1:B:557:GLU:H	0.90	0.86
1:B:469:GLN:NE2	1:B:557:GLU:H	1.74	0.86
1:A:364:ALA:H	1:A:384:ASN:ND2	1.73	0.85
1:A:469:GLN:NE2	1:A:557:GLU:H	1.75	0.85
1:A:603:ARG:HH11	1:A:603:ARG:HB3	1.41	0.84
1:B:769:LYS:HG3	1:B:770:ILE:N	1.90	0.83
1:B:449:THR:H	1:B:958:ASN:HD21	1.25	0.83
1:B:24:ASP:HB3	1:B:27:ALA:HB2	1.59	0.81
1:B:769:LYS:CG	1:B:770:ILE:H	1.91	0.81
1:A:1072:LYS:HE2	1:A:1072:LYS:HA	1.63	0.81
1:A:838:LYS:O	1:A:842:LYS:HG2	1.81	0.80
1:A:958:ASN:HD22	1:A:958:ASN:H	1.28	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:LEU:O	1:A:795:GLU:HG2	1.81	0.80
1:A:724:GLN:H	1:A:724:GLN:NE2	1.81	0.79
1:A:863:GLN:HA	1:A:863:GLN:HE21	1.47	0.79
1:A:469:GLN:HE22	1:A:557:GLU:N	1.78	0.79
1:A:920:ILE:HB	1:A:921:PRO:HD3	1.65	0.78
1:B:267:LYS:HE2	1:B:267:LYS:HA	1.64	0.78
1:B:705:LEU:HD11	1:B:773:LYS:HA	1.67	0.77
1:B:725:ALA:O	1:B:730:HIS:HB3	1.86	0.76
1:A:724:GLN:H	1:A:724:GLN:HE21	1.30	0.76
1:A:454:ASN:HB3	1:A:457:ASN:HD21	1.50	0.75
1:B:783:LYS:O	1:B:787:GLU:HG2	1.86	0.74
1:B:127:ASN:H	1:B:127:ASN:HD22	1.32	0.74
1:A:52:GLU:CD	1:A:52:GLU:H	1.90	0.74
1:A:688:LYS:HD2	2:C:4:DC:N4	2.03	0.74
1:B:26:LYS:HG2	1:B:847:THR:HG21	1.69	0.74
1:A:127:ASN:HD22	1:A:127:ASN:H	1.35	0.73
1:A:1001:PRO:HG2	1:A:1002:GLU:OE2	1.88	0.73
1:B:469:GLN:HE22	1:B:557:GLU:N	1.76	0.72
2:C:5:DC:H2"	2:C:6:DA:H5'	1.70	0.72
1:A:367:LEU:HD23	1:A:367:LEU:H	1.54	0.72
1:A:714:ILE:HG22	1:A:719:ALA:HB2	1.70	0.72
1:B:718:MET:HE3	1:B:722:GLY:HA2	1.71	0.71
1:A:603:ARG:HB3	1:A:603:ARG:NH1	2.05	0.71
1:B:523:LEU:O	1:B:526:ARG:HG3	1.91	0.70
1:B:65:ARG:O	1:B:69:GLU:HG3	1.92	0.70
1:B:213:LYS:HE3	1:B:292:GLU:OE2	1.91	0.70
1:B:700:ARG:NE	1:B:723:LYS:HE3	2.07	0.69
1:A:1091:PHE:HE2	1:A:1095:LEU:HD23	1.58	0.69
1:B:769:LYS:O	1:B:770:ILE:HB	1.90	0.69
1:A:267:LYS:HD3	1:A:267:LYS:N	2.07	0.69
1:A:752:LYS:HZ2	1:A:752:LYS:HB2	1.57	0.68
1:B:918:ALA:O	1:B:921:PRO:HD2	1.93	0.67
1:B:700:ARG:CZ	1:B:723:LYS:HG3	2.25	0.67
1:B:995:ASP:CG	1:B:998:LYS:HG2	2.14	0.67
1:A:597:LYS:NZ	1:A:602:HIS:HD2	1.91	0.67
1:A:454:ASN:HB3	1:A:457:ASN:ND2	2.09	0.67
1:A:207:VAL:HG11	1:A:905:VAL:HG21	1.76	0.67
1:A:267:LYS:HD3	1:A:267:LYS:H	1.61	0.66
1:A:360:GLU:HG2	1:A:516:VAL:HG11	1.78	0.66
1:A:968:ASN:HD21	1:A:1060:MET:H	1.44	0.65
1:A:454:ASN:HD22	1:A:457:ASN:ND2	1.93	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:724:GLN:NE2	1:A:724:GLN:N	2.43	0.65
1:B:178:VAL:HG21	1:B:194:VAL:HA	1.77	0.65
1:B:920:ILE:HB	1:B:921:PRO:HD3	1.78	0.65
1:A:546:ASP:OD2	1:A:548:SER:HB3	1.97	0.65
1:A:584:ASN:HA	1:A:587:LYS:HD2	1.78	0.65
1:B:700:ARG:HE	1:B:723:LYS:HE3	1.61	0.65
1:B:868:ASN:OD1	1:B:869:LEU:HD22	1.96	0.65
1:B:603:ARG:HB3	1:B:603:ARG:NH1	2.09	0.64
1:B:336:GLN:HE21	1:B:417:TYR:N	1.91	0.64
1:B:401:VAL:HG12	1:B:408:ILE:HG13	1.78	0.64
1:B:336:GLN:NE2	1:B:417:TYR:H	1.90	0.63
1:B:767:LYS:HD2	1:B:768:GLY:H	1.62	0.63
1:B:234:ILE:HB	1:B:235:PRO:HD3	1.79	0.63
1:A:616:THR:HG23	1:A:668:ILE:HD11	1.80	0.63
1:A:830:MET:O	1:A:834:ARG:HG2	1.99	0.63
1:A:855:THR:OG1	1:A:858:GLU:HG3	1.99	0.63
1:A:496:LYS:HB3	1:A:497:PRO:HD3	1.80	0.62
1:B:421:ARG:HD2	2:D:7:DA:H5"	1.82	0.62
1:A:653:ASP:CB	1:A:668:ILE:HG23	2.30	0.62
1:A:816:LEU:HD13	1:A:983:VAL:HG21	1.81	0.62
1:B:89:TYR:CZ	1:B:284:ILE:HD11	2.35	0.62
1:A:791:HIS:HA	1:A:795:GLU:HG3	1.82	0.62
1:A:791:HIS:HA	1:A:795:GLU:CG	2.29	0.62
1:B:1045:ILE:HD11	1:B:1098:ARG:NH2	2.14	0.61
1:A:178:VAL:HG21	1:A:194:VAL:HG13	1.82	0.61
1:A:402:ARG:HA	1:A:408:ILE:HG22	1.82	0.61
1:A:1091:PHE:CE2	1:A:1095:LEU:HD23	2.36	0.61
1:B:514:ASN:H	1:B:514:ASN:HD22	1.48	0.61
1:B:127:ASN:HD22	1:B:127:ASN:N	1.98	0.61
1:B:715:SER:HB3	1:B:718:MET:HB3	1.83	0.61
1:B:848:TRP:CH2	1:B:850:LYS:HA	2.35	0.61
1:A:778:LYS:CE	1:A:778:LYS:H	2.12	0.61
2:C:4:DC:H2"	2:C:5:DC:OP2	2.00	0.61
1:A:958:ASN:H	1:A:958:ASN:ND2	1.98	0.61
1:A:1099:LYS:C	1:A:1099:LYS:HD3	2.21	0.61
1:B:597:LYS:NZ	1:B:602:HIS:HD2	1.99	0.61
1:B:715:SER:HB3	1:B:718:MET:CB	2.31	0.61
1:B:304:PHE:CD2	1:B:310:PRO:HG3	2.37	0.60
1:B:449:THR:H	1:B:958:ASN:ND2	1.97	0.60
1:B:675:ILE:HD11	1:B:685:ILE:HG12	1.82	0.60
1:A:1015:ASP:OD1	1:A:1016:GLN:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:THR:HG22	1:B:250:THR:O	2.01	0.60
1:B:421:ARG:HD2	2:D:7:DA:C5'	2.32	0.60
1:B:1045:ILE:HD12	1:B:1094:GLU:HG3	1.84	0.60
1:B:178:VAL:HG21	1:B:194:VAL:HG13	1.84	0.60
1:A:189:LEU:HD22	1:A:193:LEU:HD23	1.85	0.59
1:A:336:GLN:HE21	1:A:417:TYR:N	1.92	0.59
1:B:173:LYS:HD2	1:B:197:PHE:O	2.03	0.59
1:A:393:GLN:HG2	1:A:431:TYR:HB2	1.84	0.58
1:A:654:ILE:C	1:A:655:ASN:HD22	2.06	0.58
1:A:430:LYS:HE3	1:A:431:TYR:CE2	2.39	0.58
1:A:724:GLN:HE21	1:A:724:GLN:N	2.01	0.58
1:B:603:ARG:NH1	1:B:608:ASN:OD1	2.37	0.58
1:A:297:VAL:HG12	1:A:298:ASN:ND2	2.19	0.58
1:A:88:ARG:HG3	1:A:283:PRO:HB2	1.86	0.58
1:B:364:ALA:N	1:B:384:ASN:HD21	1.85	0.58
1:B:496:LYS:HB3	1:B:497:PRO:HD3	1.85	0.57
1:B:159:GLY:HA2	1:B:210:LEU:HD21	1.85	0.57
1:B:995:ASP:OD2	1:B:998:LYS:HG2	2.04	0.57
1:A:267:LYS:N	1:A:267:LYS:CD	2.67	0.57
1:A:371:LEU:C	1:A:372:LEU:HD12	2.25	0.57
1:B:260:SER:HA	1:B:263:ASP:O	2.05	0.56
1:A:267:LYS:H	1:A:267:LYS:CD	2.18	0.56
1:A:336:GLN:NE2	1:A:417:TYR:H	1.92	0.56
1:B:598:THR:HG22	1:B:1066:PRO:HD3	1.88	0.56
1:B:810:VAL:O	1:B:814:GLU:HG3	2.05	0.56
1:B:89:TYR:CZ	1:B:290:ALA:HB3	2.41	0.56
1:A:778:LYS:H	1:A:778:LYS:HE3	1.69	0.56
1:B:603:ARG:HH11	1:B:603:ARG:CB	2.14	0.56
1:B:1016:GLN:O	1:B:1020:ALA:HB2	2.06	0.56
1:A:113:THR:HG22	1:A:114:LYS:HG3	1.89	0.55
2:D:4:DC:H2"	2:D:5:DC:OP2	2.07	0.55
1:A:234:ILE:HB	1:A:235:PRO:HD3	1.88	0.55
1:A:399:GLU:OE1	1:A:399:GLU:HA	2.07	0.55
1:B:317:LEU:HG	1:B:318:ARG:NH1	2.22	0.55
1:A:82:ASN:HD22	1:A:82:ASN:C	2.10	0.55
1:A:213:LYS:HE3	1:A:292:GLU:OE1	2.07	0.55
1:A:1096:GLU:OE2	1:A:1096:GLU:HA	2.07	0.55
1:A:649:LEU:HB3	1:A:650:PHE:CD1	2.41	0.55
1:A:1025:ILE:C	1:A:1025:ILE:HD12	2.27	0.55
1:A:52:GLU:N	1:A:52:GLU:OE1	2.40	0.55
1:A:653:ASP:HB3	1:A:668:ILE:HG23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:778:LYS:H	1:A:778:LYS:CD	2.20	0.54
1:B:332:LEU:O	1:B:336:GLN:HG3	2.07	0.54
1:B:705:LEU:HD11	1:B:773:LYS:CA	2.34	0.54
1:B:735:LEU:O	1:B:739:LEU:HD13	2.06	0.54
1:A:603:ARG:NH1	1:A:608:ASN:OD1	2.41	0.54
1:B:620:MET:HG3	1:B:664:LEU:HD12	1.90	0.54
1:B:829:ASP:O	1:B:833:GLN:HG3	2.07	0.54
1:A:1034:ARG:NH1	1:A:1034:ARG:HB2	2.22	0.54
1:B:725:ALA:C	1:B:727:SER:H	2.11	0.54
1:A:653:ASP:HB2	1:A:668:ILE:HG23	1.89	0.54
1:A:886:GLU:O	2:C:8:DA:H4'	2.08	0.54
1:B:1001:PRO:HG2	1:B:1002:GLU:OE2	2.08	0.54
1:A:600:ASN:ND2	1:A:600:ASN:H	2.06	0.53
1:A:127:ASN:HD22	1:A:127:ASN:N	1.98	0.53
1:A:1014:TYR:HA	1:A:1017:ARG:CZ	2.39	0.53
1:A:259:MET:CB	1:A:266:ASN:HD22	2.21	0.53
1:A:1061:ALA:O	1:A:1062:ALA:HB2	2.08	0.53
1:B:597:LYS:HE2	1:B:602:HIS:HB2	1.91	0.53
1:A:714:ILE:CG2	1:A:719:ALA:HB2	2.38	0.53
1:A:863:GLN:HA	1:A:863:GLN:NE2	2.19	0.53
1:B:1005:GLU:HG2	1:B:1009:LYS:NZ	2.24	0.53
1:B:918:ALA:C	1:B:921:PRO:HD2	2.29	0.53
1:A:649:LEU:HD13	1:A:737:ARG:NH2	2.24	0.53
1:B:749:VAL:HG13	1:B:762:THR:CG2	2.39	0.53
1:B:769:LYS:O	1:B:770:ILE:CB	2.57	0.53
1:A:816:LEU:CD1	1:A:983:VAL:HG21	2.38	0.52
1:A:700:ARG:O	1:A:704:VAL:HG23	2.09	0.52
1:A:818:LYS:O	1:A:822:ILE:HG13	2.10	0.52
1:A:465:LEU:N	1:A:483:MET:HE1	2.24	0.52
1:B:639:GLN:NE2	1:B:744:THR:CG2	2.73	0.52
1:B:655:ASN:HD21	1:B:665:LYS:HE3	1.75	0.52
1:A:178:VAL:HG21	1:A:194:VAL:HA	1.91	0.52
1:A:795:GLU:HB2	1:A:796:PRO:CD	2.40	0.52
1:B:700:ARG:NH2	1:B:723:LYS:HG3	2.25	0.52
1:A:633:ASN:CG	1:A:636:ILE:HG12	2.30	0.52
1:A:603:ARG:HH11	1:A:603:ARG:CB	2.16	0.52
1:B:520:ASN:HD21	1:B:527:LYS:NZ	2.09	0.51
1:B:668:ILE:HD12	1:B:669:ALA:N	2.25	0.51
1:A:175:ALA:HB1	1:A:186:GLN:HG3	1.91	0.51
1:B:347:VAL:O	1:B:351:GLU:HG3	2.11	0.51
1:A:1012:LEU:HD11	1:A:1025:ILE:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:VAL:HG21	1:A:40:LEU:HD21	1.91	0.51
1:A:858:GLU:O	1:A:862:ILE:HG13	2.11	0.51
1:B:82:ASN:C	1:B:82:ASN:HD22	2.12	0.51
1:A:752:LYS:HA	1:A:752:LYS:HZ1	1.75	0.51
1:B:767:LYS:CE	1:B:769:LYS:HE2	2.41	0.51
1:A:440:ARG:O	1:A:444:LEU:HD13	2.11	0.51
1:A:563:ASN:HD21	1:A:929:ASP:HB3	1.76	0.51
1:B:249:SER:O	1:B:250:THR:HB	2.11	0.51
1:A:185:ASP:OD2	1:A:187:ALA:HB3	2.10	0.50
1:B:678:TYR:O	1:B:921:PRO:HG3	2.11	0.50
1:B:816:LEU:HD13	1:B:983:VAL:HG21	1.92	0.50
1:B:322:VAL:HG22	1:B:872:MET:CE	2.41	0.50
1:B:855:THR:OG1	1:B:858:GLU:HG3	2.11	0.50
1:B:293:GLU:HA	1:B:299:PRO:CG	2.41	0.50
1:A:1061:ALA:O	1:A:1062:ALA:CB	2.60	0.50
1:B:185:ASP:HB3	1:B:188:LEU:HD12	1.94	0.50
1:A:463:PHE:HA	1:A:957:LEU:HD13	1.94	0.50
1:B:190:PRO:HD2	1:B:193:LEU:HD22	1.92	0.50
1:B:269:THR:O	2:D:11:DA:H5'	2.12	0.50
1:A:587:LYS:NZ	1:A:607:ASP:OD2	2.45	0.49
1:B:514:ASN:HD22	1:B:514:ASN:N	2.09	0.49
1:B:671:ASN:HB3	1:B:672:PRO:HD3	1.94	0.49
1:B:1079:THR:O	1:B:1083:GLN:HG3	2.12	0.49
1:A:454:ASN:HD21	1:A:456:ASN:HB2	1.76	0.49
1:A:968:ASN:ND2	1:A:1060:MET:H	2.08	0.49
1:B:47:ARG:HD2	1:B:294:ALA:O	2.12	0.49
1:B:750:PRO:HD3	1:B:788:ASN:OD1	2.11	0.49
1:A:369:LYS:NZ	1:A:369:LYS:HB3	2.27	0.49
1:A:371:LEU:HD13	1:A:371:LEU:O	2.12	0.49
1:B:351:GLU:HG2	1:B:395:PHE:CE2	2.46	0.49
1:B:767:LYS:HE2	1:B:769:LYS:HE2	1.94	0.49
1:A:342:VAL:HG11	1:A:408:ILE:HD12	1.93	0.49
1:B:777:ILE:HG22	1:B:782:LEU:HG	1.93	0.49
1:B:1061:ALA:O	1:B:1062:ALA:HB2	2.13	0.49
1:B:730:HIS:O	1:B:733:GLU:HB3	2.13	0.49
1:A:358:ILE:HD12	1:A:391:TYR:CE1	2.47	0.49
1:A:65:ARG:O	1:A:69:GLU:HG3	2.12	0.49
1:A:88:ARG:HD3	1:A:283:PRO:HD2	1.94	0.49
1:A:269:THR:O	2:C:11:DA:H5'	2.12	0.49
1:A:370:GLU:O	1:A:370:GLU:HG3	2.12	0.49
1:A:367:LEU:HB2	1:A:372:LEU:CD2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:ASN:OD1	1:A:636:ILE:HG12	2.13	0.48
1:A:721:PHE:HA	1:A:724:GLN:NE2	2.28	0.48
1:B:16:TYR:O	1:B:35:LYS:CE	2.61	0.48
1:B:649:LEU:HD13	1:B:737:ARG:NH2	2.28	0.48
1:B:714:ILE:CG1	1:B:719:ALA:HB2	2.42	0.48
1:A:176:LYS:HD2	2:C:5:DC:OP2	2.13	0.48
1:A:190:PRO:HG2	1:A:193:LEU:HB2	1.96	0.48
1:B:737:ARG:HA	1:B:740:LYS:HE2	1.95	0.48
1:B:968:ASN:HD21	1:B:1060:MET:H	1.62	0.48
1:B:767:LYS:HD2	1:B:768:GLY:N	2.27	0.48
1:B:69:GLU:HB3	1:B:74:LYS:O	2.12	0.48
1:B:113:THR:HG22	1:B:114:LYS:HG3	1.96	0.48
1:B:284:ILE:HD13	1:B:284:ILE:O	2.14	0.48
1:B:316:GLN:NE2	1:B:421:ARG:HA	2.29	0.48
1:A:6:GLU:O	1:A:6:GLU:HG2	2.13	0.48
1:A:665:LYS:O	1:A:668:ILE:HG12	2.14	0.48
1:B:767:LYS:HE2	1:B:769:LYS:HG2	1.95	0.48
1:A:304:PHE:HB3	1:A:308:ASP:O	2.14	0.48
1:A:259:MET:HB3	1:A:266:ASN:HD22	1.79	0.48
1:B:802:THR:HG23	1:B:810:VAL:HG21	1.96	0.48
1:A:262:ILE:N	1:A:262:ILE:HD12	2.29	0.47
1:A:597:LYS:HZ1	1:A:602:HIS:HD2	1.61	0.47
1:A:639:GLN:NE2	1:A:744:THR:OG1	2.47	0.47
1:B:304:PHE:CG	1:B:310:PRO:HG3	2.49	0.47
1:A:655:ASN:HB2	1:A:663:GLU:HB3	1.96	0.47
1:B:207:VAL:HG11	1:B:905:VAL:HG21	1.96	0.47
1:B:182:THR:HA	1:B:270:ILE:CD1	2.45	0.47
1:B:694:THR:HG21	1:B:782:LEU:HD21	1.97	0.47
1:A:72:THR:O	1:A:74:LYS:HG3	2.14	0.47
1:A:653:ASP:OD1	1:A:667:GLY:HA3	2.14	0.47
1:A:319:ASN:HD22	1:A:319:ASN:HA	1.56	0.47
1:A:1014:TYR:HA	1:A:1017:ARG:NE	2.30	0.47
1:A:1094:GLU:OE2	1:A:1098:ARG:NH1	2.47	0.47
1:B:565:PRO:HA	1:B:677:ILE:HG12	1.97	0.47
1:A:565:PRO:HA	1:A:677:ILE:HG12	1.97	0.47
1:A:627:ARG:NH2	1:A:640:ILE:HG22	2.30	0.47
1:B:82:ASN:ND2	1:B:85:VAL:H	2.12	0.47
1:A:343:HIS:HE1	1:A:537:GLU:OE2	1.98	0.47
1:B:444:LEU:N	1:B:444:LEU:HD23	2.30	0.47
1:A:325:THR:OG1	1:A:328:GLN:HG3	2.15	0.47
1:A:600:ASN:H	1:A:600:ASN:HD22	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:683:ARG:HH21	2:D:3:DT:H5"	1.80	0.47
1:A:367:LEU:HD23	1:A:367:LEU:N	2.27	0.46
1:A:778:LYS:H	1:A:778:LYS:HD2	1.80	0.46
1:A:833:GLN:O	1:A:837:GLU:HG3	2.16	0.46
1:B:70:LEU:HD13	1:B:70:LEU:O	2.14	0.46
1:A:620:MET:HG2	1:A:664:LEU:HD12	1.96	0.46
1:A:1099:LYS:HD3	1:A:1099:LYS:O	2.15	0.46
1:A:377:ALA:O	1:A:381:GLU:HG3	2.15	0.46
1:A:793:PHE:O	1:A:796:PRO:HG2	2.15	0.46
1:A:767:LYS:HD2	1:A:767:LYS:HA	1.77	0.46
1:B:628:SER:O	1:B:631:ALA:HB2	2.16	0.46
1:B:693:VAL:O	1:B:697:ILE:HG13	2.16	0.46
1:B:701:MET:O	1:B:772:PRO:HB2	2.14	0.46
1:A:210:LEU:HB3	1:A:239:ALA:HB1	1.98	0.46
1:A:385:ARG:HD3	1:A:386:SER:N	2.30	0.46
1:A:778:LYS:HZ2	1:A:781:GLN:NE2	2.13	0.46
1:A:633:ASN:OD1	1:A:635:PRO:HD2	2.15	0.46
1:B:176:LYS:HE3	2:D:5:DC:OP2	2.16	0.46
1:B:178:VAL:CG2	1:B:194:VAL:HG13	2.45	0.46
1:A:171:ALA:HB2	2:C:7:DA:N7	2.30	0.46
1:A:250:THR:O	1:A:250:THR:HG22	2.16	0.46
1:A:664:LEU:HB3	1:A:668:ILE:CD1	2.46	0.46
1:B:1057:ILE:HD12	1:B:1057:ILE:N	2.30	0.46
1:A:629:ASN:N	1:A:629:ASN:HD22	2.12	0.46
1:B:304:PHE:HB3	1:B:308:ASP:O	2.16	0.46
1:B:421:ARG:HG3	4:D:152:HOH:O	2.16	0.46
1:A:739:LEU:HB3	1:A:767:LYS:HZ1	1.81	0.46
1:B:127:ASN:H	1:B:127:ASN:ND2	2.09	0.46
1:B:816:LEU:CD1	1:B:983:VAL:HG21	2.46	0.46
1:A:810:VAL:O	1:A:814:GLU:HG3	2.16	0.45
1:B:965:ARG:HG2	4:B:1333:HOH:O	2.16	0.45
1:B:1061:ALA:O	1:B:1062:ALA:CB	2.64	0.45
1:A:778:LYS:NZ	1:A:781:GLN:NE2	2.64	0.45
1:A:836:GLN:HA	1:A:836:GLN:OE1	2.16	0.45
1:A:981:LYS:O	1:A:985:GLU:HG3	2.16	0.45
1:A:364:ALA:N	1:A:384:ASN:HD21	1.96	0.45
1:A:791:HIS:HA	1:A:795:GLU:HG2	1.97	0.45
1:A:1008:GLY:O	1:A:1012:LEU:HB2	2.16	0.45
1:A:514:ASN:HD22	1:A:514:ASN:H	1.65	0.45
1:B:336:GLN:O	1:B:414:HIS:HD2	1.99	0.45
1:A:191:GLU:HG2	1:A:375:ASN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ARG:HD2	2:C:7:DA:H5"	1.98	0.45
1:A:783:LYS:O	1:A:787:GLU:HG2	2.16	0.45
1:A:1053:VAL:HG12	1:A:1054:ASN:N	2.30	0.45
1:B:597:LYS:HZ1	1:B:602:HIS:HD2	1.63	0.45
1:B:715:SER:O	1:B:716:ALA:HB3	2.16	0.45
1:B:343:HIS:CD2	1:B:345:PRO:HD2	2.52	0.45
1:A:26:LYS:HD3	1:A:847:THR:HG21	1.99	0.45
1:B:355:LYS:HD2	1:B:388:GLU:HG3	1.98	0.45
1:B:890:VAL:HG11	1:B:909:ILE:HD11	1.98	0.45
1:A:217:TYR:OH	1:A:292:GLU:HA	2.17	0.45
1:A:257:VAL:HG12	1:A:259:MET:CE	2.47	0.45
1:B:196:GLN:O	1:B:199:THR:HG22	2.17	0.45
1:B:322:VAL:HG22	1:B:872:MET:HE1	1.99	0.45
1:B:639:GLN:NE2	1:B:744:THR:HG22	2.32	0.45
1:B:749:VAL:HG13	1:B:762:THR:HG21	1.99	0.45
1:A:54:PRO:O	1:A:58:VAL:HG23	2.17	0.45
1:A:135:LEU:O	1:A:138:VAL:HG22	2.17	0.45
1:A:89:TYR:CZ	1:A:290:ALA:HB3	2.52	0.44
1:B:16:TYR:O	1:B:35:LYS:HE2	2.17	0.44
1:A:194:VAL:O	1:A:198:ASP:HB2	2.17	0.44
1:A:918:ALA:O	1:A:921:PRO:HD2	2.17	0.44
1:A:1017:ARG:HG2	1:A:1017:ARG:HH11	1.82	0.44
1:A:318:ARG:O	1:A:421:ARG:NH1	2.50	0.44
1:A:598:THR:HG22	1:A:1066:PRO:HD3	1.99	0.44
1:A:651:LEU:HA	1:A:652:PRO:HD3	1.86	0.44
1:B:715:SER:HB3	1:B:718:MET:HB2	2.00	0.44
1:A:174:ASP:OD1	1:A:176:LYS:HB3	2.17	0.44
1:A:654:ILE:HD11	1:A:668:ILE:HG21	2.00	0.44
1:A:821:GLN:O	1:A:825:VAL:HG23	2.17	0.44
1:B:197:PHE:CD1	1:B:272:LEU:HD21	2.53	0.44
1:A:336:GLN:O	1:A:414:HIS:HD2	2.01	0.44
1:A:609:ASN:HB3	1:A:613:GLN:HB3	1.99	0.44
1:B:724:GLN:HA	1:B:724:GLN:OE1	2.17	0.44
1:A:196:GLN:O	1:A:272:LEU:HD21	2.18	0.44
1:A:317:LEU:HB3	4:C:29:HOH:O	2.17	0.44
1:B:135:LEU:O	1:B:138:VAL:HG22	2.18	0.44
1:B:563:ASN:HD21	1:B:929:ASP:HB3	1.81	0.44
1:B:725:ALA:C	1:B:727:SER:N	2.71	0.44
1:A:37:SER:HB3	1:A:231:THR:HG22	1.99	0.44
1:A:45:LYS:HE3	4:A:1232:HOH:O	2.18	0.44
1:A:1057:ILE:N	1:A:1057:ILE:HD12	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1053:VAL:HG11	1:A:1075:LEU:HD12	1.99	0.43
1:A:100:ALA:O	1:A:104:ARG:HG3	2.18	0.43
1:A:118:LYS:O	1:A:122:GLN:HG3	2.18	0.43
1:A:444:LEU:HG	1:A:553:PRO:HB2	2.00	0.43
1:A:471:LEU:O	1:A:472:ASP:HB2	2.18	0.43
1:A:12:ILE:HA	1:A:40:LEU:HD11	1.99	0.43
1:A:370:GLU:HA	1:A:773:LYS:HE2	1.99	0.43
1:A:372:LEU:HD23	1:A:380:LEU:HD12	2.00	0.43
1:B:444:LEU:HB3	4:B:1167:HOH:O	2.17	0.43
1:B:725:ALA:HB1	1:B:730:HIS:CD2	2.52	0.43
1:A:386:SER:O	1:A:390:SER:HB2	2.19	0.43
1:A:762:THR:HB	1:A:764:THR:HG22	2.01	0.43
1:B:455:GLN:HG2	1:B:460:PHE:CZ	2.53	0.43
1:B:714:ILE:HG12	1:B:719:ALA:HB2	2.00	0.43
1:B:942:ALA:HA	1:B:943:PRO:HD3	1.90	0.43
1:A:671:ASN:HB3	1:A:672:PRO:HD3	2.01	0.43
1:A:1058:ASP:HB2	1:A:1066:PRO:HB3	1.99	0.43
1:B:321:ALA:HB2	1:B:910:TYR:HE2	1.84	0.43
1:A:752:LYS:NZ	1:A:752:LYS:CB	2.81	0.43
1:B:585:ILE:HG12	1:B:590:LEU:HD23	2.01	0.43
1:B:725:ALA:O	1:B:727:SER:N	2.52	0.43
1:B:1005:GLU:HG2	1:B:1009:LYS:HZ3	1.84	0.43
1:A:89:TYR:O	1:A:93:MET:HG2	2.19	0.43
1:A:304:PHE:CD2	1:A:310:PRO:HG3	2.53	0.43
1:A:319:ASN:N	1:A:320:PRO:HD3	2.33	0.43
1:A:597:LYS:HZ3	1:A:602:HIS:HD2	1.65	0.43
1:A:711:ASP:OD1	1:A:714:ILE:HG12	2.18	0.43
1:A:1034:ARG:HG3	4:A:1249:HOH:O	2.18	0.43
1:B:318:ARG:NE	2:D:7:DA:C5	2.87	0.43
1:B:848:TRP:CZ3	1:B:850:LYS:HA	2.53	0.43
1:A:303:MET:CE	1:A:397:VAL:HG13	2.48	0.43
1:A:432:ASN:HB2	1:A:433:PRO:CD	2.49	0.43
1:A:664:LEU:HB3	1:A:668:ILE:HD11	2.01	0.43
1:B:174:ASP:O	1:B:177:ASP:HB2	2.18	0.43
1:B:369:LYS:O	1:B:371:LEU:N	2.52	0.43
1:A:156:VAL:O	1:A:160:LEU:HG	2.19	0.43
1:A:967:ALA:O	1:A:971:VAL:HG23	2.19	0.43
1:A:1053:VAL:O	1:A:1055:LEU:HD13	2.17	0.43
1:B:438:LEU:C	1:B:438:LEU:HD23	2.38	0.43
1:B:609:ASN:OD1	1:B:613:GLN:HG2	2.19	0.43
1:A:454:ASN:ND2	1:A:457:ASN:ND2	2.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:ASN:HD22	1:B:384:ASN:HA	1.64	0.42
1:A:514:ASN:HD22	1:A:514:ASN:N	2.17	0.42
1:A:752:LYS:HZ2	1:A:752:LYS:CB	2.27	0.42
1:A:766:ALA:HB2	1:A:781:GLN:CD	2.40	0.42
1:A:955:ILE:HD13	1:A:963:ALA:HB3	2.01	0.42
1:B:685:ILE:HD12	1:B:798:ARG:HD3	2.01	0.42
1:B:705:LEU:O	1:B:709:ALA:HB2	2.20	0.42
1:A:367:LEU:HB2	1:A:372:LEU:HD21	2.02	0.42
1:B:343:HIS:HE1	1:B:537:GLU:OE2	2.02	0.42
1:B:627:ARG:NH1	1:B:627:ARG:HG2	2.35	0.42
1:A:306:GLY:O	1:A:414:HIS:HE1	2.03	0.42
1:B:728:GLU:OE2	1:B:728:GLU:HA	2.18	0.42
1:B:767:LYS:CE	1:B:769:LYS:HG2	2.50	0.42
1:A:752:LYS:HA	1:A:752:LYS:NZ	2.35	0.42
1:A:795:GLU:HB2	1:A:796:PRO:HD3	2.02	0.42
1:B:634:MET:HB2	1:B:635:PRO:HD3	2.01	0.42
1:A:739:LEU:CB	1:A:767:LYS:HZ1	2.33	0.42
1:B:620:MET:CG	1:B:664:LEU:HD12	2.50	0.42
1:B:710:LYS:O	1:B:711:ASP:HB2	2.20	0.42
1:B:821:GLN:HE22	1:B:914:GLN:NE2	2.18	0.42
1:A:369:LYS:O	1:A:370:GLU:HB3	2.20	0.41
1:A:399:GLU:OE1	1:A:402:ARG:NH1	2.53	0.41
1:B:37:SER:HB3	1:B:231:THR:HG22	2.02	0.41
1:B:165:THR:O	1:B:169:ASN:ND2	2.53	0.41
1:B:192:GLY:HA3	1:B:378:LYS:HB3	2.02	0.41
1:B:292:GLU:HG3	1:B:299:PRO:HB3	2.01	0.41
1:A:321:ALA:HB2	1:A:910:TYR:HE1	1.85	0.41
1:A:675:ILE:HD11	1:A:685:ILE:HG12	2.01	0.41
1:B:374:ASP:O	1:B:378:LYS:HG2	2.20	0.41
1:B:1048:LYS:HE2	1:B:1048:LYS:HB3	1.91	0.41
1:A:432:ASN:HB2	1:A:433:PRO:HD2	2.03	0.41
1:B:20:VAL:HG23	1:B:138:VAL:O	2.20	0.41
1:B:432:ASN:HB2	1:B:433:PRO:CD	2.50	0.41
1:A:1098:ARG:NE	1:A:1098:ARG:HA	2.36	0.41
1:B:184:ILE:HG12	4:B:1445:HOH:O	2.19	0.41
1:A:241:GLU:OE2	1:A:898:ASN:HB2	2.20	0.41
1:A:1041:LEU:O	1:A:1045:ILE:HG12	2.21	0.41
1:B:319:ASN:HD22	1:B:319:ASN:HA	1.51	0.41
1:A:118:LYS:HE3	1:A:118:LYS:HB2	1.93	0.41
1:A:343:HIS:CE1	1:A:537:GLU:OE2	2.74	0.41
1:A:1053:VAL:HG21	1:A:1087:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ASN:N	1:B:127:ASN:ND2	2.67	0.41
1:B:368:ASN:C	1:B:368:ASN:ND2	2.73	0.41
1:B:467:LEU:O	1:B:471:LEU:HD23	2.21	0.41
1:A:512:PRO:HB2	1:A:514:ASN:ND2	2.36	0.41
1:A:1053:VAL:HG13	1:A:1075:LEU:HG	2.03	0.41
1:B:184:ILE:HD13	1:B:262:ILE:HG21	2.02	0.41
1:B:368:ASN:C	1:B:368:ASN:HD22	2.23	0.41
1:B:454:ASN:HB3	1:B:457:ASN:ND2	2.35	0.41
1:A:741:ASP:HA	1:A:744:THR:HG22	2.02	0.41
1:A:1041:LEU:HD22	1:A:1041:LEU:HA	1.91	0.41
1:B:733:GLU:O	1:B:736:ALA:HB3	2.21	0.41
1:A:173:LYS:HD2	1:A:197:PHE:O	2.20	0.41
1:A:870:ALA:HB2	1:A:989:LYS:HD3	2.03	0.41
1:B:173:LYS:HA	1:B:177:ASP:OD1	2.20	0.41
1:B:250:THR:O	1:B:250:THR:CG2	2.69	0.41
1:A:16:TYR:O	1:A:35:LYS:CE	2.69	0.40
1:A:683:ARG:HG3	1:A:683:ARG:HH11	1.86	0.40
1:A:626:LEU:O	1:A:630:TYR:HD1	2.04	0.40
1:A:655:ASN:HD22	1:A:655:ASN:N	2.15	0.40
1:A:715:SER:OG	1:A:718:MET:HB2	2.22	0.40
1:A:369:LYS:HE2	1:A:377:ALA:HB1	2.03	0.40
1:A:845:ASP:HA	1:A:846:PRO:HD2	1.85	0.40
1:A:886:GLU:HG3	1:A:908:SER:HB3	2.04	0.40
1:B:24:ASP:HB3	1:B:27:ALA:CB	2.42	0.40
1:B:293:GLU:HA	1:B:299:PRO:HG2	2.03	0.40
1:B:317:LEU:HD21	1:B:318:ARG:HH12	1.86	0.40
1:B:421:ARG:HD2	2:D:7:DA:H5'	2.01	0.40
1:A:267:LYS:HE2	1:A:267:LYS:HB2	1.76	0.40
1:A:471:LEU:HD12	1:A:471:LEU:HA	1.96	0.40
1:A:753:ARG:O	1:A:754:LYS:HB2	2.22	0.40
1:A:1034:ARG:HB2	1:A:1034:ARG:HH11	1.86	0.40
1:A:1075:LEU:HD21	1:A:1086:GLU:HG2	2.03	0.40
1:A:1091:PHE:C	1:A:1091:PHE:CD2	2.95	0.40
1:A:178:VAL:CG2	1:A:194:VAL:HG13	2.51	0.40
1:A:490:LEU:HD23	1:A:495:LEU:HD11	2.03	0.40
1:A:652:PRO:HD3	4:A:1481:HOH:O	2.21	0.40
1:A:831:PHE:O	1:A:835:VAL:HG23	2.21	0.40
1:A:853:PHE:CG	1:A:854:LEU:N	2.89	0.40
1:A:918:ALA:C	1:A:921:PRO:HD2	2.42	0.40
1:B:932:MET:HE2	1:B:1060: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	1093/1117 (98%)	1050 (96%)	35 (3%)	8 (1%)	22	16
1	B	1092/1117 (98%)	1053 (96%)	30 (3%)	9 (1%)	19	13
All	All	2185/2234 (98%)	2103 (96%)	65 (3%)	17 (1%)	19	13

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	370	GLU
1	A	1062	ALA
1	B	770	ILE
1	B	1062	ALA
1	A	369	LYS
1	A	371	LEU
1	A	779	GLY
1	B	724	GLN
1	B	728	GLU
1	A	666	ARG
1	B	370	GLU
1	B	727	SER
1	B	666	ARG
1	B	726	ALA
1	A	1014	TYR
1	A	1018	GLU
1	B	711	ASP

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	916/934 (98%)	878 (96%)	38 (4%)	30	28
1	B	915/934 (98%)	889 (97%)	26 (3%)	43	44
All	All	1831/1868 (98%)	1767 (96%)	64 (4%)	36	35

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	GLU
1	A	52	GLU
1	A	70	LEU
1	A	82	ASN
1	A	88	ARG
1	A	127	ASN
1	A	163	ARG
1	A	210	LEU
1	A	267	LYS
1	A	319	ASN
1	A	367	LEU
1	A	444	LEU
1	A	447	LYS
1	A	471	LEU
1	A	483	MET
1	A	494	ASN
1	A	514	ASN
1	A	520	ASN
1	A	603	ARG
1	A	613	GLN
1	A	623	LEU
1	A	648	ASP
1	A	708	ARG
1	A	724	GLN
1	A	740	LYS
1	A	752	LYS
1	A	771	ASN
1	A	778	LYS
1	A	817	GLN
1	A	838	LYS
1	A	886	GLU
1	A	958	ASN
1	A	1004	LEU
1	A	1017	ARG

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Mol	Chain	Res	Type
1	A	1036	LEU
1	A	1041	LEU
1	A	1091	PHE
1	A	1095	LEU
1	B	52	GLU
1	B	82	ASN
1	B	124	THR
1	B	127	ASN
1	B	163	ARG
1	B	210	LEU
1	B	265	ASP
1	B	284	ILE
1	B	319	ASN
1	B	368	ASN
1	B	444	LEU
1	B	483	MET
1	B	514	ASN
1	B	520	ASN
1	B	603	ARG
1	B	623	LEU
1	B	662	LEU
1	B	670	LYS
1	B	677	ILE
1	B	771	ASN
1	B	838	LYS
1	B	886	GLU
1	B	909	ILE
1	B	1036	LEU
1	B	1041	LEU
1	B	1050	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	127	ASN
1	A	150	GLN
1	A	169	ASN
1	A	266	ASN
1	A	298	ASN
1	A	316	GLN
1	A	319	ASN

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Mol	Chain	Res	Type
1	A	324	ASN
1	A	336	GLN
1	A	343	HIS
1	A	348	GLN
1	A	373	ASN
1	A	384	ASN
1	A	414	HIS
1	A	455	GLN
1	A	457	ASN
1	A	469	GLN
1	A	494	ASN
1	A	506	ASN
1	A	514	ASN
1	A	520	ASN
1	A	563	ASN
1	A	600	ASN
1	A	602	HIS
1	A	629	ASN
1	A	639	GLN
1	A	655	ASN
1	A	724	GLN
1	A	771	ASN
1	A	781	GLN
1	A	815	GLN
1	A	817	GLN
1	A	823	GLN
1	A	863	GLN
1	A	867	ASN
1	A	954	ASN
1	A	958	ASN
1	A	968	ASN
1	A	1035	ASN
1	A	1038	ASN
1	A	1059	GLN
1	B	82	ASN
1	B	122	GLN
1	B	127	ASN
1	B	150	GLN
1	B	169	ASN
1	B	186	GLN
1	B	196	GLN
1	B	255	ASN

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Mol	Chain	Res	Type
1	B	316	GLN
1	B	319	ASN
1	B	324	ASN
1	B	336	GLN
1	B	343	HIS
1	B	348	GLN
1	B	368	ASN
1	B	376	HIS
1	B	384	ASN
1	B	414	HIS
1	B	456	ASN
1	B	457	ASN
1	B	469	GLN
1	B	514	ASN
1	B	520	ASN
1	B	563	ASN
1	B	602	HIS
1	B	629	ASN
1	B	639	GLN
1	B	655	ASN
1	B	771	ASN
1	B	781	GLN
1	B	786	GLN
1	B	815	GLN
1	B	817	GLN
1	B	833	GLN
1	B	892	ASN
1	B	893	GLN
1	B	914	GLN
1	B	954	ASN
1	B	958	ASN
1	B	968	ASN
1	B	1027	ASN
1	B	1035	ASN
1	B	1047	HIS
1	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 (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)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	2HP	A	1106	-	4,4,4	2.03	3 (75%)	6,6,6	0.32	0
3	2HP	B	1106	-	4,4,4	2.00	2 (50%)	6,6,6	0.44	0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1106	2HP	P-O1	2.59	1.56	1.50
3	A	1106	2HP	P-O2	2.56	1.62	1.54
3	A	1106	2HP	P-O1	2.38	1.56	1.50
3	B	1106	2HP	P-O2	2.26	1.61	1.54
3	A	1106	2HP	P-O3	2.06	1.60	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	1095/1117 (98%)	0.27	67 (6%) 21 20	9, 25, 61, 75	0
1	B	1094/1117 (97%)	0.26	67 (6%) 21 20	10, 23, 58, 81	0
2	C	20/36 (55%)	0.33	2 (10%) 7 6	25, 36, 85, 86	0
2	D	21/36 (58%)	0.16	2 (9%) 8 7	19, 30, 70, 78	0
All	All	2230/2306 (96%)	0.26	138 (6%) 20 19	9, 24, 61, 86	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	725	ALA	11.9
1	A	1014	TYR	6.6
1	A	708	ARG	5.6
1	B	708	ARG	5.5
1	A	658	GLU	5.4
1	B	766	ALA	5.1
1	B	768	GLY	5.1
1	A	714	ILE	5.1
1	A	369	LYS	5.0
1	A	184	ILE	4.9
1	A	265	ASP	4.6
1	B	723	LYS	4.6
1	B	8	LEU	4.5
1	B	769	LYS	4.2
1	A	710	LYS	4.1
1	B	6	GLU	4.1
1	B	724	GLN	4.1
1	B	709	ALA	4.0
1	A	661	ALA	4.0
1	A	767	LYS	4.0
1	B	713	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	718	MET	3.9
1	A	371	LEU	3.9
1	A	1018	GLU	3.8
2	C	4	DC	3.8
1	A	7	GLU	3.8
1	A	726	ALA	3.8
1	B	719	ALA	3.8
1	B	726	ALA	3.8
1	B	711	ASP	3.7
1	B	7	GLU	3.7
1	B	712	PRO	3.7
1	B	188	LEU	3.7
1	A	8	LEU	3.6
1	B	1018	GLU	3.6
1	A	1098	ARG	3.6
1	A	766	ALA	3.6
1	B	729	ALA	3.6
1	A	711	ASP	3.6
1	B	264	PRO	3.5
1	A	712	PRO	3.5
1	B	764	THR	3.5
1	A	264	PRO	3.4
1	A	1019	ASN	3.3
1	B	707	ALA	3.3
1	B	5	THR	3.3
1	A	188	LEU	3.3
1	A	677	ILE	3.3
1	B	192	GLY	3.2
1	B	265	ASP	3.2
1	B	715	SER	3.2
1	A	723	LYS	3.2
1	A	730	HIS	3.1
2	D	23	DT	3.1
1	B	730	HIS	3.1
1	B	714	ILE	3.1
1	B	1014	TYR	3.1
1	A	185	ASP	3.0
1	B	185	ASP	3.0
1	A	267	LYS	3.0
1	B	767	LYS	3.0
1	A	367	LEU	2.9
1	A	657	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	370	GLU	2.9
1	B	195	GLU	2.9
1	B	770	ILE	2.8
1	B	191	GLU	2.8
2	C	23	DT	2.8
1	A	372	LEU	2.8
1	A	175	ALA	2.8
1	A	1015	ASP	2.8
1	A	28	GLU	2.7
1	B	172	ILE	2.7
1	B	1019	ASN	2.7
1	A	1020	ALA	2.7
1	A	770	ILE	2.7
1	A	717	ALA	2.7
1	B	262	ILE	2.6
1	B	705	LEU	2.6
1	A	775	TYR	2.6
1	B	194	VAL	2.6
1	B	754	LYS	2.6
1	A	1100	GLN	2.6
1	B	659	ASN	2.6
1	B	775	TYR	2.6
1	A	678	TYR	2.6
1	B	1096	GLU	2.6
1	A	768	GLY	2.5
1	A	728	GLU	2.5
1	A	713	ASN	2.5
1	B	722	GLY	2.5
1	B	755	GLY	2.4
1	B	28	GLU	2.4
1	A	707	ALA	2.4
1	A	266	ASN	2.4
1	A	725	ALA	2.4
1	B	910	TYR	2.4
1	A	74	LYS	2.3
1	B	184	ILE	2.3
1	A	910	TYR	2.3
1	B	1095	LEU	2.3
1	A	709	ALA	2.3
1	A	729	ALA	2.3
1	A	183	GLY	2.3
1	A	659	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	683	ARG	2.3
1	B	26	LYS	2.2
1	B	281	PHE	2.2
1	A	261	GLU	2.2
1	A	370	GLU	2.2
1	A	1005	GLU	2.2
1	A	755	GLY	2.2
1	B	720	MET	2.2
1	A	189	LEU	2.2
1	A	10	GLU	2.2
1	B	267	LYS	2.2
2	D	3	DT	2.2
1	B	70	LEU	2.2
1	B	1015	ASP	2.2
1	B	260	SER	2.2
1	B	780	GLU	2.1
1	A	731	ALA	2.1
1	A	719	ALA	2.1
1	B	261	GLU	2.1
1	A	765	GLY	2.1
1	B	74	LYS	2.1
1	B	710	LYS	2.1
1	B	545	GLU	2.1
1	A	705	LEU	2.1
1	B	187	ALA	2.1
1	A	191	GLU	2.0
1	A	727	SER	2.0
1	A	656	LEU	2.0
1	B	658	GLU	2.0
1	B	743	GLU	2.0
1	A	192	GLY	2.0
1	A	73	GLU	2.0
1	B	657	GLY	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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	2HP	B	1106	5/5	0.94	0.14	34,34,37,38	0
3	2HP	A	1106	5/5	0.96	0.14	27,28,30,32	0

6.5 Other polymers

There are no such residues in this entry.