



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:49 PM UTC

PDB ID : 3C2P / pdb_00003c2p
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

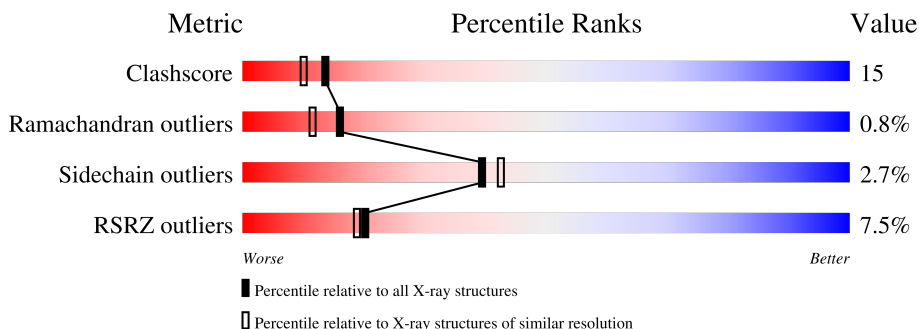
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	33	12% 39% 21% 39%
1	D	33	3% 39% 18% 42%
2	A	1117	7% 70% 25% • •
2	B	1117	7% 69% 26% • •

2 Entry composition

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

Continued on next page...

Continued from previous page...

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

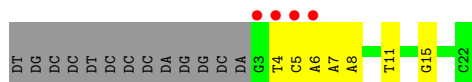
- Molecule 3 is water.

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

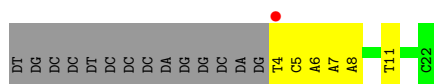
3 Residue-property plots

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.

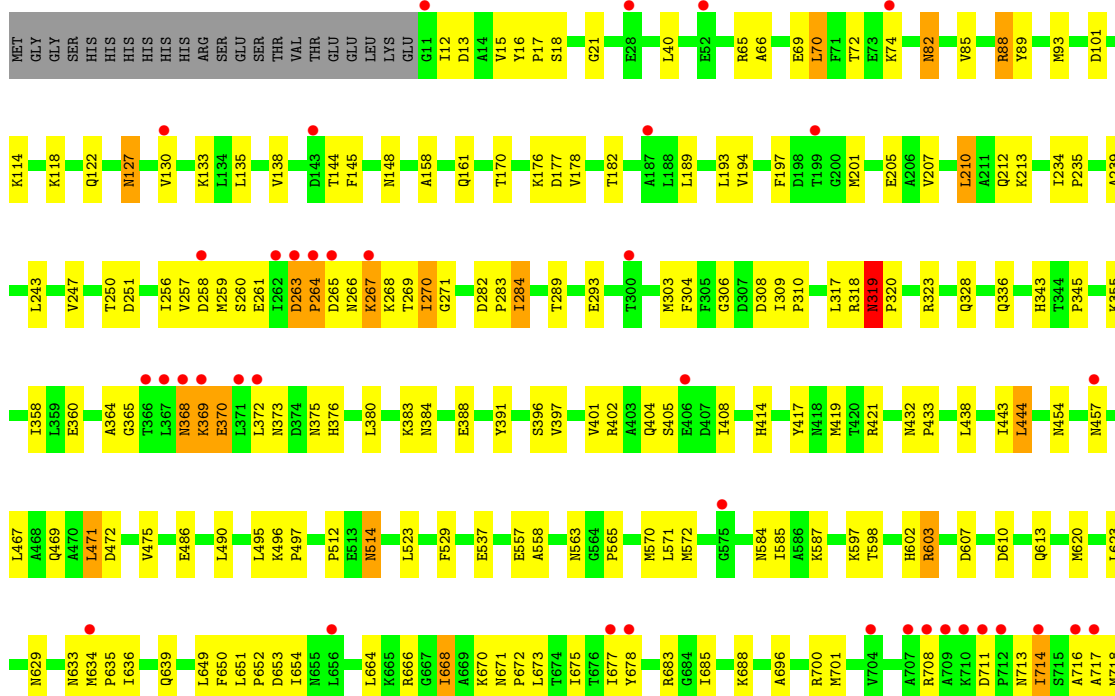
• Molecule 1: P1 Promoter DNA

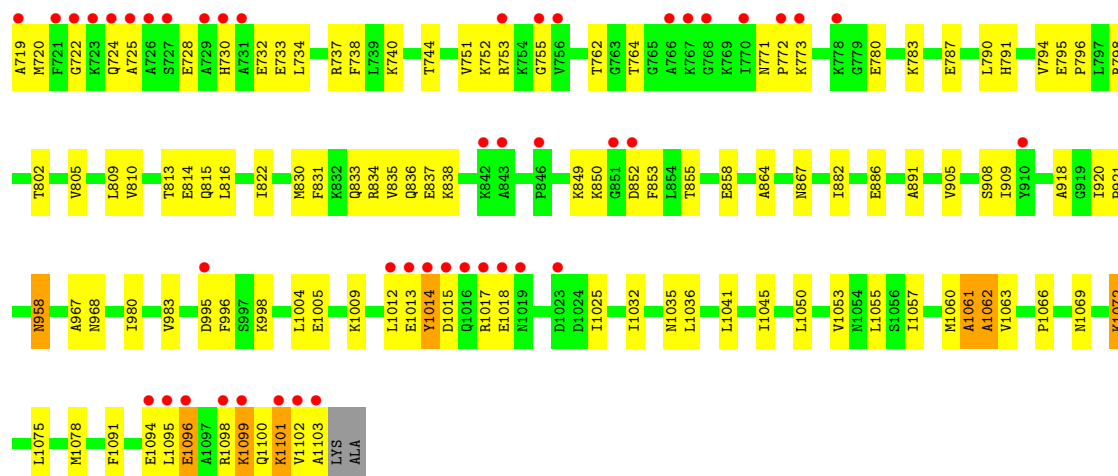


• Molecule 1: P1 Promoter DNA

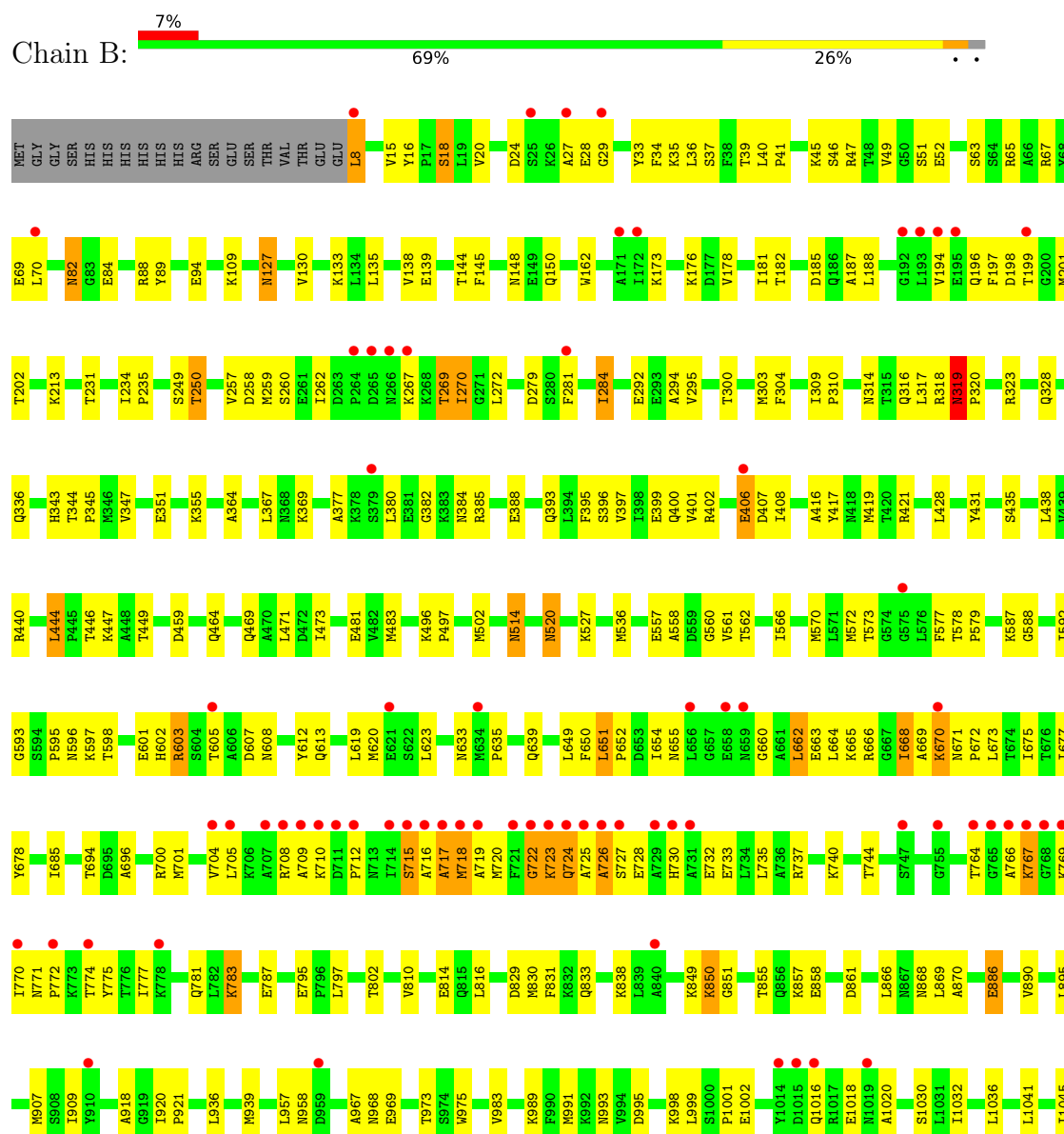


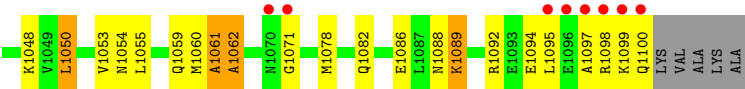
• Molecule 2: Virion RNA polymerase





• Molecule 2: Virion RNA polymerase





4 Data and refinement statistics

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 50.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	83.1 (50.00-2.00) 83.6 (50.00-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.256 (Not available) , (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 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

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	0.28	0/463	0.71	0/713
1	D	0.26	0/438	0.70	0/674
2	A	0.41	0/8560	0.91	22/11579 (0.2%)
2	B	0.42	0/8565	0.93	29/11585 (0.3%)
All	All	0.41	0/18026	0.91	51/24551 (0.2%)

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	852	ASP	N-CA-C	-10.55	97.44	110.41
2	B	660	GLY	N-CA-C	-9.53	101.84	115.27
2	B	1097	ALA	N-CA-C	-9.39	101.51	113.16
2	A	1061	ALA	N-CA-C	9.35	121.91	110.41
2	B	722	GLY	N-CA-C	-8.51	102.39	115.66
2	B	148	ASN	N-CA-C	-8.24	97.47	109.59
2	B	558	ALA	N-CA-C	-7.41	97.19	108.67
2	B	1061	ALA	N-CA-C	7.27	120.37	110.55
2	B	270	ILE	N-CA-C	7.07	118.06	108.17
2	A	558	ALA	N-CA-C	-7.02	97.78	108.67
2	A	263	ASP	CA-C-N	6.82	128.36	119.84
2	A	263	ASP	C-N-CA	6.82	128.36	119.84
2	B	18	SER	N-CA-C	6.56	120.20	112.72
2	B	473	ILE	N-CA-C	-6.47	100.40	109.21
2	B	572	MET	N-CA-C	6.47	121.09	112.30
2	A	572	MET	N-CA-C	6.35	120.67	112.41
2	A	396	SER	N-CA-C	-6.28	104.52	111.36
2	B	717	ALA	N-CA-C	-6.22	105.51	113.23
2	A	270	ILE	N-CA-C	6.12	116.74	108.17
2	B	34	PHE	N-CA-C	-6.11	103.94	111.40
2	A	563	ASN	N-CA-C	6.00	118.34	111.02
2	A	21	GLY	N-CA-C	5.94	118.10	112.04
2	A	148	ASN	N-CA-C	-5.88	100.25	109.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	295	VAL	N-CA-C	5.85	116.03	110.53
2	A	251	ASP	N-CA-C	-5.83	105.66	112.89
2	B	651	LEU	CA-C-N	5.81	125.50	119.05
2	B	651	LEU	C-N-CA	5.81	125.50	119.05
2	B	1089	LYS	N-CA-C	-5.76	105.08	111.36
2	A	882	ILE	N-CA-C	5.74	116.47	110.62
2	B	718	MET	N-CA-C	-5.72	106.14	113.23
2	B	319	ASN	CA-C-N	5.66	126.92	119.84
2	B	319	ASN	C-N-CA	5.66	126.92	119.84
2	A	1063	VAL	N-CA-C	5.63	116.41	110.72
2	A	319	ASN	CA-C-N	5.56	126.79	119.84
2	A	319	ASN	C-N-CA	5.56	126.79	119.84
2	B	459	ASP	N-CA-C	-5.50	105.36	111.36
2	B	715	SER	N-CA-C	5.45	119.02	112.38
2	A	1018	GLU	N-CA-C	5.44	117.91	111.33
2	B	269	THR	N-CA-C	-5.37	99.66	108.41
2	B	1071	GLY	N-CA-C	-5.35	103.24	111.64
2	A	18	SER	N-CA-C	5.32	119.75	113.16
2	B	573	THR	N-CA-C	-5.25	100.61	108.96
2	A	523	LEU	N-CA-C	5.24	118.13	111.69
2	B	709	ALA	N-CA-C	-5.23	106.41	112.89
2	B	300	THR	N-CA-C	-5.20	107.06	113.41
2	B	396	SER	N-CA-C	-5.19	105.80	111.82
2	A	1072	LYS	N-CA-C	5.10	117.97	111.69
2	A	475	VAL	N-CA-C	5.09	119.21	111.89
2	B	957	LEU	N-CA-C	5.07	118.56	112.38
2	A	571	LEU	N-CA-C	5.06	118.60	112.23
2	B	435	SER	N-CA-C	5.04	119.56	113.41

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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	389	0	214	8	0
2	A	8431	0	8464	274	0
2	B	8436	0	8467	235	0
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	513	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 (513) 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	1.39	1.01
2:A:161:GLN:HB3	2:A:213:LYS:HZ1	1.26	0.99
2:B:469:GLN:HE22	2:B:557:GLU:H	1.02	0.97
2:B:701:MET:HE1	2:B:720:MET:HE2	1.45	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:364:ALA:H	2:A:384:ASN:HD21	1.16	0.90
2:A:158:ALA:HA	2:A:213:LYS:HZ3	1.36	0.89
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:620:MET:HE2	2:A:664:LEU:HB2	1.58	0.86
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:895:LEU:HD13	2:B:907:MET:HE3	1.61	0.83
2:B:601:GLU:O	2:B:605:THR:HG22	1.78	0.82
2:B:303:MET:HE3	2:B:400:GLN:NE2	1.96	0.80
2:B:267:LYS:HE2	2:B:267:LYS:HA	1.63	0.79
2:A:161:GLN:CB	2:A:213:LYS:HZ1	1.93	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:82:ASN:HD22	2:A:82:ASN:C	1.92	0.77
2:B:395:PHE:O	2:B:399:GLU:HG3	1.85	0.76
2:B:995:ASP:CG	2:B:998:LYS:HG2	2.11	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
2:A:303:MET:HE1	2:A:397:VAL:HG13	1.70	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: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:1032:ILE:O	2:B:1036:LEU:HD13	1.91	0.71
2:A:15:VAL:C	2:A:17:PRO:HD3	2.17	0.70
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:654:ILE:C	2:B:655:ASN:HD22	2.01	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:170:THR:HG22	2:A:201:MET:HE3	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:B:830:MET:HE3	2:B:999:LEU:HD23	1.75	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:B:144:THR:HG22	2:B:145:PHE:N	1.99	0.66
2:A:161:GLN:HB3	2:A:213:LYS:CE	2.25	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:B:701:MET:HE1	2:B:720:MET:CE	2.25	0.62
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:158:ALA:HA	2:A:213:LYS:HZ2	1.66	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:416:ALA:C	2:B:428:LEU:HD23	2.28	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:162:TRP:CZ2	2:B:201:MET:HE1	2.37	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:1075:LEU:HA	2:A:1078:MET:HE3	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:266:ASN:HD22	2:A:266:ASN:C	2.12	0.57
2:B:718:MET:HE3	2:B:722:GLY:HA2	1.86	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
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:B:701:MET:O	2:B:704:VAL:HG12	2.05	0.56
2:B:520:ASN:HD21	2:B:527:LYS:HZ2	1.53	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:671:ASN:C	2:A:671:ASN:HD22	2.15	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:82:ASN:C	2:B:82:ASN:HD22	2.14	0.54
2:B:918:ALA:C	2:B:921:PRO:HD2	2.33	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:B:176:LYS:C	2:B:176:LYS:HD3	2.32	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:A:833:GLN:O	2:A:837:GLU:HG3	2.08	0.54
2:B:715:SER:O	2:B:716:ALA:HB3	2.07	0.54
2:B:1078:MET:HE2	2:B:1082:GLN:HB3	1.89	0.54
2:A:82:ASN:C	2:A:82:ASN:ND2	2.63	0.54
2:A:918:ALA:C	2:A:921:PRO:HD2	2.32	0.54
2:A:816:LEU:CD1	2:A:983:VAL:HG21	2.38	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
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:502:MET:CE	2:B:536:MET:HE2	2.39	0.53
2:B:464:GLN:CB	2:B:483:MET:HE1	2.39	0.53
2:B:303:MET:HE3	2:B:400:GLN:HE21	1.73	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:443:ILE:C	2:A:444:LEU:HD22	2.34	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:201:MET:HE2	2:A:205:GLU:HG2	1.92	0.52
2:A:720:MET:HE1	2:A:738:PHE:CE2	2.43	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:DC:H5'	2:A:921:PRO:HG2	1.92	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:263:ASP:O	2:A:263:ASP:CG	2.53	0.51
2:A:289:THR:O	2:A:293:GLU:HG3	2.10	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: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:752:LYS:HZ2	2:A:755:GLY:HA2	1.73	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: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
2:A:514:ASN:HD22	2:A:514:ASN:H	1.57	0.50
2:A:170:THR:CG2	2:A:201:MET:HE3	2.42	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: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:A:740:LYS:HD2	2:A:740:LYS:C	2.37	0.50
2:A:89:TYR:O	2:A:93:MET:HG2	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:597:LYS:HZ1	2:A:602:HIS:HD2	1.60	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:A:1041:LEU:C	2:A:1041:LEU:HD13	2.37	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: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:257:VAL:HG23	2:A:257:VAL:O	2.12	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:328:GLN:HB3	2:B:419:MET:HE3	1.95	0.48
2:B:868:ASN:OD1	2:B:869:LEU:HD22	2.13	0.48
2:A:176:LYS:HD3	2:A:176:LYS:C	2.38	0.48
2:B:319:ASN:HD22	2:B:319:ASN:HA	1.53	0.48
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:A:771:ASN:C	2:A:773:LYS:H	2.22	0.48
2:B:135:LEU:O	2:B:138:VAL:HG22	2.13	0.48
2:B:895:LEU:CD1	2:B:907:MET:HE3	2.39	0.48
2:B:909:ILE:C	2:B:909:ILE:HD12	2.38	0.48
2:A:370:GLU:HA	2:A:773:LYS:HZ3	1.77	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:A:718:MET:HE1	2:A:728:GLU:HA	1.96	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:158:ALA:CA	2:A:213:LYS:HZ2	2.25	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:771:ASN:C	2:A:771:ASN:HD22	2.21	0.47
2:A:795:GLU:HB2	2:A:796:PRO:CD	2.45	0.47
2:B:446:THR:C	2:B:447:LYS:HG3	2.39	0.47
2:B:597:LYS:HE2	2:B:602:HIS:HB2	1.96	0.47
2:A:701:MET:HE2	2:A:701:MET:HA	1.95	0.47
2:B:28:GLU:CD	2:B:29:GLY:N	2.72	0.47
2:A:633:ASN:CG	2:A:636:ILE:HG12	2.39	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:1025:ILE:C	2:A:1025:ILE:HD12	2.39	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: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:328:GLN:HB3	2:A:419:MET:HE3	1.97	0.46
2:A:514:ASN:HD22	2:A:514:ASN:N	2.13	0.46
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:438:LEU:C	2:B:438:LEU:HD23	2.40	0.46
2:B:704:VAL:HG23	2:B:719:ALA:CB	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:752:LYS:HZ3	2:A:755:GLY:HA2	1.80	0.46
2:B:704:VAL:O	2:B:708:ARG:HG2	2.15	0.46
2:B:991:MET:HE2	2:B:1030:SER:HA	1.98	0.46
2:A:258:ASP:OD2	2:A:261:GLU:HG2	2.14	0.46
2:A:370:GLU:HB2	2:A:773:LYS:HZ3	1.80	0.46
2:A:257:VAL:HG23	2:A:259:MET:HE3	1.98	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:A:771:ASN:C	2:A:771:ASN:ND2	2.74	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:266:ASN:ND2	2:A:266:ASN:C	2.74	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:B:464:GLN:HB2	2:B:483:MET:HE1	1.97	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:481:GLU:H	2:B:481:GLU:CD	2.23	0.45
2:B:514:ASN:HD22	2:B:514:ASN:N	2.12	0.45
2:B:939:MET:HE1	2:B:969:GLU:HB3	1.98	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:127:ASN:H	2:A:127:ASN:ND2	2.01	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:158:ALA:C	2:A:213:LYS:HZ2	2.24	0.45
2:A:343:HIS:HE1	2:A:537:GLU:OE2	2.00	0.45
2:A:718:MET:HE2	2:A:728:GLU:HA	1.99	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
2:A:454:ASN:HB3	2:A:457:ASN:ND2	2.32	0.45
2:B:344:THR:HB	2:B:345:PRO:HD3	1.97	0.45
2:B:561:VAL:O	2:B:562:THR:C	2.59	0.45
2:B:587:LYS:NZ	2:B:607:ASP:OD2	2.42	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:303:MET:HE1	2:B:397:VAL:HA	1.99	0.45
2:B:560:GLY:HA2	2:B:1059:GLN:O	2.16	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:A:1102:VAL:O	2:A:1103:ALA:C	2.59	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: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:A:66:ALA:O	2:A:70:LEU:HD22	2.18	0.44
2:A:93:MET:HE2	2:A:93:MET:HA	1.98	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:A:1091:PHE:C	2:A:1091:PHE:CD2	2.96	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:774:THR:O	2:B:775:TYR:C	2.60	0.43
2:A:370:GLU:CA	2:A:773:LYS:HZ3	2.31	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:700:ARG:NH2	2:B:723:LYS:CD	2.70	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: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: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: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: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:849:LYS:O	2:B:850:LYS:C	2.61	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1002:GLU:CD	2:B:1002:GLU:H	2.27	0.42
2:A:135:LEU:O	2:A:138:VAL:HG22	2.19	0.42
2:A:161:GLN:HB3	2:A:213:LYS:HZ2	1.77	0.42
2:B:259:MET:HA	2:B:259:MET:HE2	2.02	0.42
2:B:969:GLU:O	2:B:973:THR:HG23	2.20	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:711:ASP:C	2:A:713:ASN:H	2.28	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: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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:816:LEU:HD13	2:A:983:VAL:HG21	2.03	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:A:762:THR:C	2:A:764:THR:H	2.30	0.40
2:B:620:MET:HG3	2:B:664:LEU:HD12	2.03	0.40
2:A:514:ASN:ND2	2:A:514:ASN:C	2.79	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: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:B:715:SER:C	2:B:717:ALA:H	2.28	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

5.3.1 Protein backbone

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%)	16	11
2	B	1091/1117 (98%)	1050 (96%)	33 (3%)	8 (1%)	18	14
All	All	2182/2234 (98%)	2098 (96%)	67 (3%)	17 (1%)	16	11

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

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%)	889 (97%)	24 (3%)	40	44
2	B	914/934 (98%)	889 (97%)	25 (3%)	39	42
All	All	1827/1868 (98%)	1778 (97%)	49 (3%)	39	42

All (49) 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	210	LEU
2	A	212	GLN
2	A	267	LYS
2	A	284	ILE
2	A	309	ILE
2	A	319	ASN
2	A	368	ASN
2	A	444	LEU
2	A	471	LEU
2	A	472	ASP
2	A	486	GLU
2	A	514	ASN
2	A	603	ARG
2	A	623	LEU
2	A	668	ILE
2	A	714	ILE
2	A	836	GLN
2	A	838	LYS
2	A	958	ASN
2	A	1096	GLU
2	B	8	LEU
2	B	52	GLU
2	B	70	LEU
2	B	82	ASN
2	B	94	GLU
2	B	127	ASN
2	B	250	THR
2	B	284	ILE
2	B	319	ASN
2	B	406	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	444	LEU
2	B	471	LEU
2	B	514	ASN
2	B	520	ASN
2	B	603	ARG
2	B	623	LEU
2	B	662	LEU
2	B	668	ILE
2	B	670	LYS
2	B	783	LYS
2	B	795	GLU
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 (85) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	44	GLN
2	A	82	ASN
2	A	127	ASN
2	A	150	GLN
2	A	186	GLN
2	A	212	GLN
2	A	225	ASN
2	A	266	ASN
2	A	298	ASN
2	A	316	GLN
2	A	319	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	454	ASN
2	A	455	GLN
2	A	457	ASN
2	A	464	GLN
2	A	469	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	494	ASN
2	A	514	ASN
2	A	563	ASN
2	A	602	HIS
2	A	613	GLN
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
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	384	ASN
2	B	404	GLN
2	B	414	HIS
2	B	457	ASN
2	B	469	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	506	ASN
2	B	514	ASN
2	B	520	ASN
2	B	602	HIS
2	B	629	ASN
2	B	639	GLN
2	B	655	ASN
2	B	730	HIS
2	B	781	GLN
2	B	786	GLN
2	B	817	GLN
2	B	833	GLN
2	B	856	GLN
2	B	892	ASN
2	B	914	GLN
2	B	954	ASN
2	B	958	ASN
2	B	968	ASN
2	B	982	ASN
2	B	1019	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	20/33 (60%)	0.85	4 (20%) 3 2	22, 42, 66, 71	0
1	D	19/33 (57%)	0.46	1 (5%) 32 31	21, 33, 52, 54	0
2	A	1093/1117 (97%)	0.43	83 (7%) 20 18	9, 25, 53, 76	0
2	B	1093/1117 (97%)	0.36	78 (7%) 22 20	9, 23, 53, 83	0
All	All	2225/2300 (96%)	0.40	166 (7%) 20 19	9, 24, 53, 83	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	726	ALA	7.8
2	B	725	ALA	6.1
2	A	1014	TYR	5.7
2	A	1103	ALA	5.2
2	A	1102	VAL	5.0
2	A	1019	ASN	4.8
2	B	659	ASN	4.6
2	A	723	LYS	4.6
2	B	1097	ALA	4.5
2	A	262	ILE	4.5
2	A	727	SER	4.5
2	B	1095	LEU	4.3
2	B	727	SER	4.3
2	A	726	ALA	4.3
2	B	716	ALA	4.2
2	B	723	LYS	4.0
2	A	1018	GLU	4.0
2	B	704	VAL	3.9
2	A	1101	LYS	3.9
2	A	1015	ASP	3.8
2	A	1094	GLU	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	722	GLY	3.7
2	B	764	THR	3.7
2	B	705	LEU	3.6
2	B	199	THR	3.6
2	B	707	ALA	3.6
2	B	172	ILE	3.5
2	B	729	ALA	3.5
2	B	171	ALA	3.5
2	B	714	ILE	3.5
2	B	721	PHE	3.5
2	A	371	LEU	3.5
2	B	710	LYS	3.5
2	B	769	LYS	3.4
2	A	768	GLY	3.4
2	A	710	LYS	3.4
2	A	842	LYS	3.3
2	B	766	ALA	3.3
2	A	729	ALA	3.3
1	C	3	DG	3.3
2	B	1099	LYS	3.3
2	B	718	MET	3.2
2	B	765	GLY	3.2
2	B	731	ALA	3.2
2	B	265	ASP	3.2
2	B	281	PHE	3.2
2	B	711	ASP	3.2
2	B	8	LEU	3.1
2	A	730	HIS	3.1
2	A	731	ALA	3.1
2	A	725	ALA	3.0
2	A	843	ALA	3.0
2	A	714	ILE	3.0
2	B	770	ILE	3.0
2	B	724	GLN	3.0
2	A	712	PRO	3.0
2	B	1014	TYR	3.0
2	B	712	PRO	2.9
2	A	753	ARG	2.9
2	A	772	PRO	2.9
2	B	719	ALA	2.9
2	A	1013	GLU	2.9
2	B	715	SER	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	724	GLN	2.8
1	C	5	DC	2.8
2	B	1015	ASP	2.8
2	A	372	LEU	2.8
2	A	846	PRO	2.8
2	A	678	TYR	2.8
2	A	708	ARG	2.7
2	A	1095	LEU	2.7
2	B	656	LEU	2.7
2	B	708	ARG	2.7
2	A	756	VAL	2.7
1	C	6	DA	2.7
1	C	4	DT	2.7
1	D	4	DT	2.7
2	A	1017	ARG	2.7
2	A	366	THR	2.7
2	B	910	TYR	2.7
2	B	717	ALA	2.6
2	B	1096	GLU	2.6
2	B	264	PRO	2.6
2	A	1023	ASP	2.6
2	A	267	LYS	2.6
2	A	719	ALA	2.6
2	B	709	ALA	2.6
2	B	195	GLU	2.6
2	A	457	ASN	2.6
2	A	707	ALA	2.6
2	A	264	PRO	2.6
2	A	721	PHE	2.6
2	A	704	VAL	2.6
2	B	575	GLY	2.6
2	A	199	THR	2.6
2	B	747	SER	2.6
2	A	1099	LYS	2.5
2	B	772	PRO	2.5
2	A	851	GLY	2.5
2	A	263	ASP	2.5
2	B	658	GLU	2.5
2	A	767	LYS	2.5
2	A	265	ASP	2.5
2	B	379	SER	2.5
2	A	1012	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	634	MET	2.5
2	B	768	GLY	2.5
2	A	995	ASP	2.4
2	B	605	THR	2.4
2	B	670	LYS	2.4
2	B	1098	ARG	2.4
2	B	621	GLU	2.4
2	A	258	ASP	2.4
2	A	28	GLU	2.3
2	B	70	LEU	2.3
2	A	1098	ARG	2.3
2	A	52	GLU	2.3
2	A	910	TYR	2.3
2	A	755	GLY	2.3
2	A	1096	GLU	2.3
2	A	300	THR	2.3
2	B	774	THR	2.3
2	B	1016	GLN	2.3
2	B	194	VAL	2.3
2	A	368	ASN	2.3
2	A	130	VAL	2.2
2	A	709	ALA	2.2
2	A	722	GLY	2.2
2	A	406	GLU	2.2
2	B	1100	GLN	2.2
2	A	770	ILE	2.2
2	A	634	MET	2.2
2	A	717	ALA	2.2
2	A	1016	GLN	2.2
2	B	25	SER	2.2
2	B	29	GLY	2.2
2	B	27	ALA	2.2
2	B	840	ALA	2.2
2	A	778	LYS	2.2
2	B	192	GLY	2.1
2	A	656	LEU	2.1
2	A	369	LYS	2.1
2	B	1019	ASN	2.1
2	A	711	ASP	2.1
2	A	575	GLY	2.1
2	B	755	GLY	2.1
2	B	1071	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	187	ALA	2.1
2	B	266	ASN	2.1
2	B	406	GLU	2.1
2	A	852	ASP	2.1
2	B	778	LYS	2.1
2	A	367	LEU	2.1
2	B	1070	ASN	2.1
2	B	730	HIS	2.1
2	A	74	LYS	2.1
2	A	766	ALA	2.1
2	B	193	LEU	2.0
2	A	143	ASP	2.0
2	A	773	LYS	2.0
2	B	767	LYS	2.0
2	A	11	GLY	2.0
2	A	677	ILE	2.0
2	A	716	ALA	2.0
2	B	959	ASP	2.0
2	B	267	LYS	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 oligosaccharides 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.