



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:22 PM UTC

PDB ID : 4DDV / pdb_00004ddv
Title : Thermotoga maritima reverse gyrase, triclinic form
Authors : Rudolph, M.G.; Klostermeier, D.
Deposited on : 2012-01-19
Resolution : 3.46 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

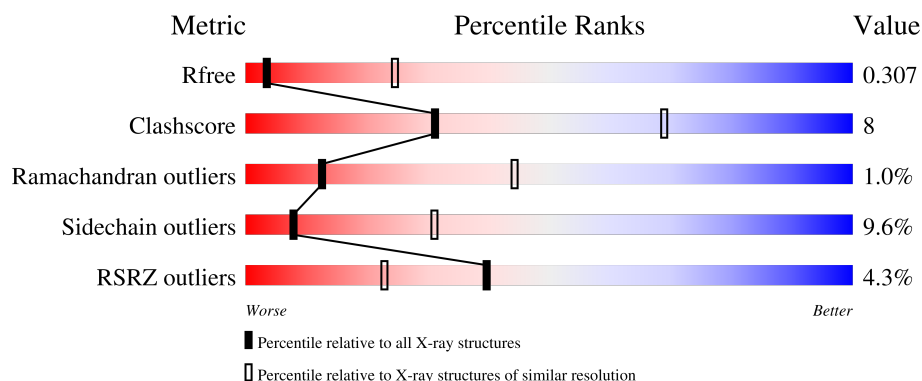
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.46 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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	A	1104	5% 74% 22% • •
1	B	1104	3% 69% 25% 5% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18064 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 Reverse gyrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1102	Total	C	N	O	S	0	0	0
			9030	5759	1563	1682	26			
1	B	1102	Total	C	N	O	S	0	0	0
			9030	5759	1563	1682	26			

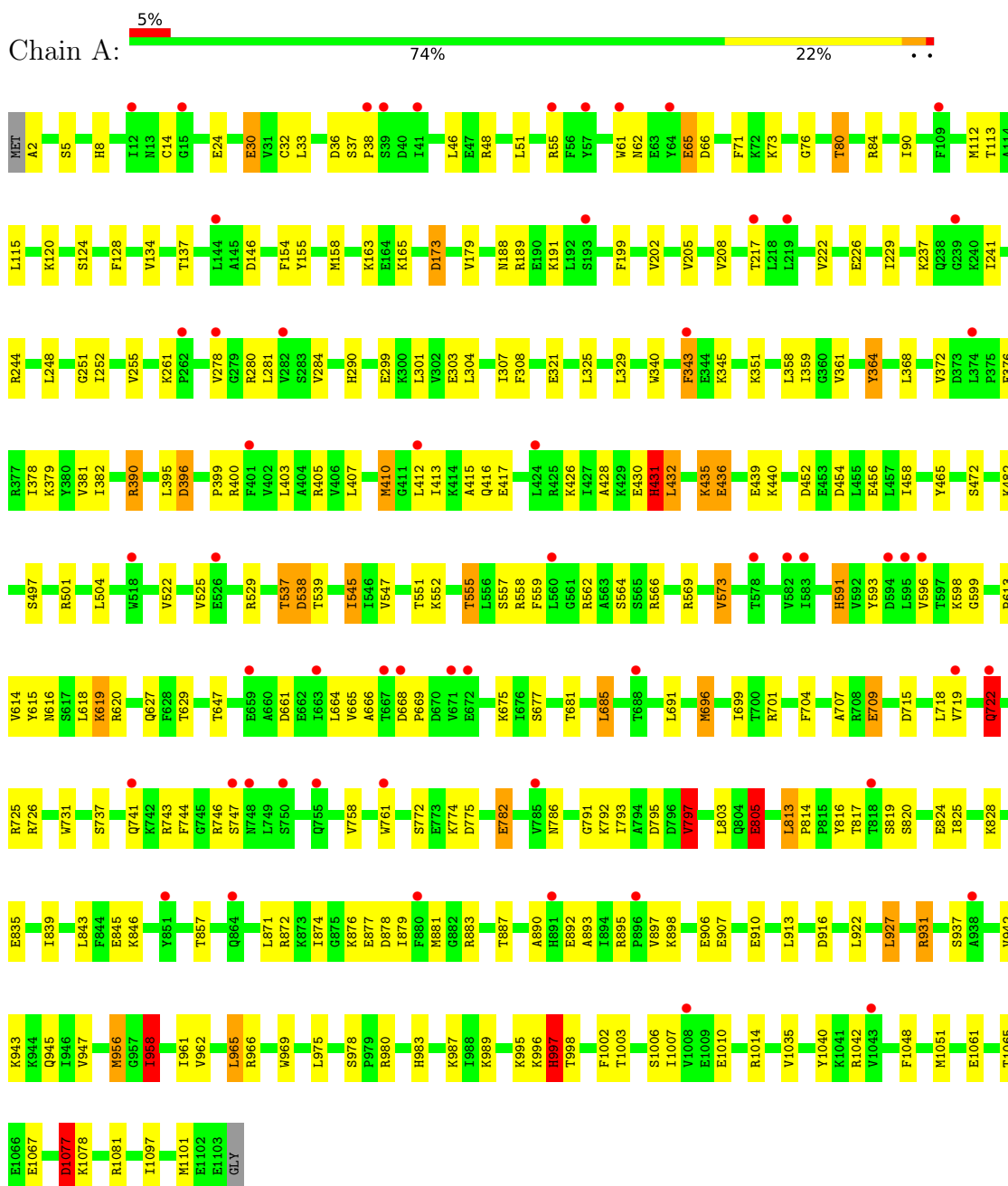
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

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: Reverse gyrase



Chain B: 3% 69% 25% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	95.71Å 101.25Å 104.43Å 113.61° 97.50° 110.42°	Depositor
Resolution (Å)	49.11 – 3.46 49.11 – 3.46	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.11-3.46) 98.3 (49.11-3.46)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.235 , 0.278 0.260 , 0.307	Depositor DCC
R_{free} test set	2069 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	82.1	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 112.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	18064	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6894e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.75	3/9191 (0.0%)	1.20	34/12356 (0.3%)
1	B	0.94	11/9191 (0.1%)	1.40	70/12356 (0.6%)
All	All	0.85	14/18382 (0.1%)	1.30	104/24712 (0.4%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	958	ILE	CG1-CD1	6.48	1.77	1.51
1	B	560	LEU	CA-C	6.35	1.60	1.52
1	B	704	PHE	CA-C	6.23	1.60	1.52
1	B	585	PHE	CA-C	-6.23	1.45	1.52
1	B	563	ALA	C-N	6.18	1.42	1.33
1	B	961	ILE	CG1-CD1	5.89	1.74	1.51
1	B	852	HIS	CA-C	5.74	1.60	1.52
1	A	696	MET	SD-CE	-5.54	1.65	1.79
1	B	933	LEU	CA-C	-5.41	1.45	1.52
1	B	37	SER	CA-C	5.29	1.59	1.52
1	B	546	ILE	CA-C	-5.25	1.46	1.52
1	B	480	LEU	CA-C	5.22	1.59	1.52
1	B	543	LEU	C-N	5.13	1.41	1.33
1	A	416	GLN	CA-C	5.02	1.57	1.52

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	670	ASP	CA-CB-CG	9.64	122.24	112.60
1	A	1048	PHE	CA-CB-CG	9.19	122.99	113.80
1	B	660	ALA	CA-C-N	8.67	132.77	120.28
1	B	660	ALA	C-N-CA	8.67	132.77	120.28
1	B	977	VAL	N-CA-CB	8.57	120.77	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	ASP	N-CA-C	-8.50	97.94	110.52
1	B	709	GLU	N-CA-C	-8.01	102.64	111.36
1	B	587	ALA	CA-C-N	7.93	132.36	120.31
1	B	587	ALA	C-N-CA	7.93	132.36	120.31
1	B	916	ASP	CA-CB-CG	7.92	120.52	112.60
1	A	538	ASP	N-CA-C	7.47	121.64	109.76
1	A	8	HIS	N-CA-C	7.38	121.38	112.38
1	B	40	ASP	CA-C-N	7.35	130.08	120.60
1	B	40	ASP	C-N-CA	7.35	130.08	120.60
1	B	174	ASP	CA-C-N	7.35	131.89	121.02
1	B	174	ASP	C-N-CA	7.35	131.89	121.02
1	A	30	GLU	CB-CG-CD	7.22	124.87	112.60
1	A	537	THR	CB-CA-C	7.21	122.02	110.19
1	A	916	ASP	CA-CB-CG	7.21	119.81	112.60
1	B	844	PHE	CA-C-N	7.04	130.42	120.28
1	B	844	PHE	C-N-CA	7.04	130.42	120.28
1	A	709	GLU	N-CA-C	-6.97	103.77	111.36
1	A	432	LEU	N-CA-C	6.81	121.34	112.89
1	A	805	GLU	CB-CG-CD	6.72	124.03	112.60
1	B	559	PHE	CA-CB-CG	6.65	120.45	113.80
1	A	722	GLN	CB-CG-CD	6.64	123.90	112.60
1	B	543	LEU	N-CA-C	6.59	119.27	109.59
1	B	29	CYS	N-CA-C	6.55	119.53	110.35
1	B	546	ILE	CA-C-N	6.47	132.24	122.92
1	B	546	ILE	C-N-CA	6.47	132.24	122.92
1	B	961	ILE	N-CA-C	6.43	115.98	106.85
1	B	396	ASP	CA-CB-CG	6.35	118.95	112.60
1	B	552	LYS	N-CA-C	-6.12	103.77	111.11
1	B	960	GLN	CA-C-N	-6.09	114.57	123.10
1	B	960	GLN	C-N-CA	-6.09	114.57	123.10
1	B	1037	GLU	CB-CG-CD	6.02	122.84	112.60
1	B	722	GLN	CB-CG-CD	6.02	122.83	112.60
1	B	475	ILE	N-CA-CB	6.00	117.84	111.00
1	B	737	SER	CA-C-N	5.95	126.42	119.94
1	B	737	SER	C-N-CA	5.95	126.42	119.94
1	A	997	HIS	N-CA-C	5.84	118.70	110.23
1	B	173	ASP	N-CA-C	5.83	123.22	110.80
1	B	599	GLY	N-CA-C	5.80	120.81	112.81
1	B	545	ILE	N-CA-CB	5.74	118.69	111.46
1	B	1048	PHE	CA-CB-CG	5.74	119.54	113.80
1	A	173	ASP	N-CA-C	5.73	123.01	110.80
1	A	887	THR	N-CA-C	-5.71	105.99	113.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	942	VAL	N-CA-CB	-5.70	100.11	111.91
1	B	961	ILE	CA-C-N	5.66	127.77	120.70
1	B	961	ILE	C-N-CA	5.66	127.77	120.70
1	B	890	ALA	N-CA-C	-5.66	104.75	111.03
1	B	887	THR	N-CA-C	-5.65	106.06	113.12
1	A	782	GLU	CB-CG-CD	5.65	122.20	112.60
1	B	644	ASP	CA-CB-CG	5.61	118.21	112.60
1	B	556	LEU	N-CA-C	-5.58	105.11	111.14
1	A	413	ILE	CB-CA-C	5.52	120.35	111.29
1	A	431	HIS	CA-C-N	5.51	130.79	121.14
1	A	431	HIS	C-N-CA	5.51	130.79	121.14
1	B	764	GLU	CA-C-N	5.48	127.63	120.28
1	B	764	GLU	C-N-CA	5.48	127.63	120.28
1	B	118	ALA	CA-C-N	5.47	128.16	120.28
1	B	118	ALA	C-N-CA	5.47	128.16	120.28
1	A	396	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	29	CYS	CA-C-N	5.43	131.91	121.54
1	B	29	CYS	C-N-CA	5.43	131.91	121.54
1	B	1047	ARG	CA-C-N	5.36	127.41	120.44
1	B	1047	ARG	C-N-CA	5.36	127.41	120.44
1	A	599	GLY	N-CA-C	5.35	120.20	112.81
1	B	997	HIS	CA-C-N	5.33	128.82	120.82
1	B	997	HIS	C-N-CA	5.33	128.82	120.82
1	B	805	GLU	CB-CG-CD	5.32	121.64	112.60
1	B	760	GLY	CA-C-N	5.31	127.71	120.54
1	B	760	GLY	C-N-CA	5.31	127.71	120.54
1	A	37	SER	N-CA-C	5.26	121.43	109.81
1	B	961	ILE	N-CA-CB	5.25	118.29	111.83
1	B	147	GLU	CA-C-N	5.20	127.25	120.28
1	B	147	GLU	C-N-CA	5.20	127.25	120.28
1	B	569	ARG	CB-CA-C	-5.20	110.16	117.23
1	A	1077	ASP	CA-CB-CG	-5.18	107.42	112.60
1	A	817	THR	N-CA-C	-5.17	102.50	109.95
1	B	586	THR	CB-CA-C	5.15	119.88	109.68
1	A	797	VAL	N-CA-CB	5.12	119.87	111.58
1	A	537	THR	N-CA-C	-5.11	100.19	108.52
1	B	58	HIS	CA-C-N	5.09	127.36	120.38
1	B	58	HIS	C-N-CA	5.09	127.36	120.38
1	A	997	HIS	CA-C-N	5.08	127.36	120.65
1	A	997	HIS	C-N-CA	5.08	127.36	120.65
1	B	817	THR	N-CA-C	-5.08	101.93	109.96
1	A	569	ARG	CB-CA-C	-5.08	110.33	117.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	400	ARG	N-CA-C	5.08	116.50	111.07
1	B	334	PHE	CA-CB-CG	5.07	118.87	113.80
1	A	252	ILE	CB-CG1-CD1	5.07	124.44	113.80
1	B	39	SER	CA-C-N	5.05	130.83	121.94
1	B	39	SER	C-N-CA	5.05	130.83	121.94
1	B	962	VAL	CA-C-O	-5.05	115.88	121.29
1	B	704	PHE	CA-C-N	5.04	127.35	120.54
1	B	704	PHE	C-N-CA	5.04	127.35	120.54
1	B	452	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	591	HIS	CA-CB-CG	5.04	118.83	113.80
1	A	38	PRO	CA-C-N	5.01	126.95	120.44
1	A	38	PRO	C-N-CA	5.01	126.95	120.44
1	A	890	ALA	N-CA-C	-5.01	105.47	111.03
1	A	452	ASP	CA-CB-CG	5.01	117.61	112.60
1	B	791	GLY	N-CA-C	5.00	125.03	113.18

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	9030	0	9187	136	0
1	B	9030	0	9187	165	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
All	All	18064	0	18374	298	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 8.

All (298) 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:A:958:ILE:CD1	1:A:958:ILE:CG1	1.77	1.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:961:ILE:CD1	1:B:961:ILE:CG1	1.74	1.56
1:B:544:LEU:HD12	1:B:584:LEU:O	1.67	0.95
1:A:14:CYS:HB3	1:A:32:CYS:SG	2.10	0.91
1:A:722:GLN:HE22	1:A:726:ARG:HB2	1.37	0.89
1:B:543:LEU:HD21	1:B:664:LEU:HD12	1.55	0.88
1:B:722:GLN:HE22	1:B:726:ARG:HB2	1.37	0.85
1:A:746:ARG:HE	1:B:426:LYS:HE2	1.40	0.85
1:B:741:GLN:HG2	1:B:747:SER:HA	1.60	0.84
1:B:555:THR:HG21	1:B:846:LYS:HA	1.61	0.83
1:B:681:THR:HG22	1:B:691:LEU:HD22	1.61	0.82
1:A:681:THR:HG22	1:A:691:LEU:HD22	1.64	0.80
1:A:412:LEU:HD21	1:A:426:LYS:HB3	1.66	0.77
1:B:555:THR:HG22	1:B:558:ARG:NH2	2.00	0.77
1:A:555:THR:HG21	1:A:846:LYS:HA	1.67	0.77
1:A:399:PRO:O	1:A:403:LEU:HD12	1.87	0.74
1:B:669:PRO:HG2	1:B:697:HIS:CD2	2.22	0.74
1:B:399:PRO:O	1:B:403:LEU:HD12	1.88	0.74
1:A:962:VAL:HG11	1:A:980:ARG:HG3	1.70	0.74
1:B:61:TRP:O	1:B:65:GLU:HG3	1.90	0.72
1:A:958:ILE:CD1	1:A:958:ILE:HA	2.18	0.72
1:A:202:VAL:HB	1:A:255:VAL:HG12	1.72	0.72
1:A:61:TRP:O	1:A:65:GLU:HG3	1.91	0.70
1:B:202:VAL:HB	1:B:255:VAL:HG12	1.72	0.70
1:B:698:GLU:O	1:B:703:GLY:HA3	1.93	0.69
1:B:722:GLN:NE2	1:B:726:ARG:HB2	2.08	0.69
1:A:80:THR:OG1	1:A:538:ASP:OD2	2.08	0.68
1:B:556:LEU:HD23	1:B:559:PHE:CZ	2.28	0.68
1:B:556:LEU:HB3	1:B:560:LEU:HD12	1.76	0.67
1:A:741:GLN:HG2	1:A:747:SER:HA	1.78	0.66
1:B:621:CYS:HA	1:B:643:ILE:HG22	1.76	0.65
1:A:722:GLN:NE2	1:A:726:ARG:HB2	2.09	0.65
1:B:573:VAL:HA	1:B:586:THR:HB	1.78	0.65
1:A:555:THR:HG22	1:A:558:ARG:NH2	2.12	0.65
1:A:620:ARG:HG3	1:A:627:GLN:HG2	1.79	0.65
1:B:178:LEU:HD12	1:B:197:PHE:HZ	1.62	0.64
1:B:556:LEU:HB3	1:B:560:LEU:CD1	2.28	0.64
1:A:772:SER:HB3	1:A:998:THR:HB	1.79	0.64
1:B:772:SER:HB3	1:B:998:THR:HB	1.79	0.64
1:B:554:GLU:O	1:B:557:SER:OG	2.16	0.64
1:A:62:ASN:HA	1:A:65:GLU:CD	2.23	0.63
1:B:944:LYS:HB3	1:B:961:ILE:HG23	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ARG:NH1	1:B:661:ASP:OD2	2.32	0.62
1:B:62:ASN:HA	1:B:65:GLU:CD	2.25	0.62
1:B:340:TRP:HB3	1:B:364:TYR:HE1	1.65	0.62
1:B:495:PHE:CZ	1:B:499:LYS:HD3	2.35	0.61
1:B:675:LYS:HG2	1:B:722:GLN:HG3	1.82	0.61
1:A:244:ARG:HD2	1:A:248:LEU:HD23	1.82	0.61
1:A:340:TRP:HB3	1:A:364:TYR:HE1	1.64	0.61
1:A:405:ARG:NH1	1:A:907:GLU:OE1	2.34	0.61
1:B:405:ARG:NH1	1:B:907:GLU:OE1	2.35	0.60
1:B:593:TYR:HB3	1:B:615:TYR:HB3	1.84	0.60
1:B:857:THR:HA	1:B:893:ALA:HB2	1.83	0.59
1:B:883:ARG:NH2	1:B:937:SER:O	2.31	0.59
1:A:857:THR:HA	1:A:893:ALA:HB2	1.85	0.59
1:B:244:ARG:HD2	1:B:248:LEU:HD23	1.84	0.59
1:B:431:HIS:HB3	1:B:436:GLU:HB3	1.84	0.59
1:A:482:LYS:O	1:A:529:ARG:NH1	2.37	0.58
1:A:675:LYS:HG2	1:A:722:GLN:HG3	1.85	0.58
1:B:762:ILE:HD13	1:B:1035:VAL:HG21	1.86	0.58
1:A:124:SER:HB3	1:A:199:PHE:HB3	1.85	0.58
1:B:576:ALA:HB3	1:B:583:ILE:HG22	1.85	0.58
1:B:665:VAL:HG11	1:B:677:SER:HA	1.86	0.58
1:A:746:ARG:NE	1:B:426:LYS:HE2	2.15	0.58
1:B:805:GLU:HG3	1:B:945:GLN:HG3	1.86	0.58
1:B:943:LYS:HB2	1:B:965:LEU:HD11	1.84	0.57
1:B:635:CYS:O	1:B:639:SER:HA	2.05	0.57
1:A:969:TRP:CH2	1:A:975:LEU:HD13	2.40	0.57
1:A:1010:GLU:OE1	1:A:1014:ARG:NH1	2.37	0.57
1:A:504:LEU:HD12	1:A:898:LYS:HE3	1.87	0.57
1:A:593:TYR:HB3	1:A:615:TYR:HB3	1.85	0.56
1:B:669:PRO:HG3	1:B:695:GLU:HB2	1.86	0.56
1:A:997:HIS:CD2	1:A:997:HIS:H	2.22	0.56
1:B:290:HIS:HD1	1:B:465:TYR:HH	1.53	0.56
1:B:782:GLU:HA	1:B:989:LYS:HE3	1.87	0.55
1:B:632:ARG:NH2	1:B:636:PRO:HB3	2.21	0.55
1:B:872:ARG:HA	1:B:877:GLU:HB3	1.87	0.55
1:B:545:ILE:HD11	1:B:583:ILE:HG13	1.87	0.55
1:A:381:VAL:HG23	1:A:472:SER:HB3	1.89	0.55
1:B:550:PRO:O	1:B:553:ALA:HB3	2.06	0.55
1:A:497:SER:O	1:A:501:ARG:HG2	2.07	0.55
1:A:699:ILE:HD12	1:A:845:GLU:HA	1.88	0.55
1:B:303:GLU:O	1:B:307:ILE:HG12	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:962:VAL:HG11	1:B:980:ARG:CZ	2.37	0.54
1:A:883:ARG:NH2	1:A:937:SER:O	2.29	0.54
1:A:816:TYR:CZ	1:A:931:ARG:HG3	2.42	0.54
1:A:872:ARG:HA	1:A:877:GLU:HB3	1.89	0.54
1:A:557:SER:HB2	1:A:562:ARG:HB2	1.88	0.54
1:B:497:SER:O	1:B:501:ARG:HG2	2.08	0.54
1:A:619:LYS:NZ	1:A:629:THR:O	2.40	0.54
1:A:782:GLU:HA	1:A:989:LYS:HE3	1.89	0.54
1:B:557:SER:HB2	1:B:562:ARG:HB2	1.90	0.54
1:A:84:ARG:NH1	1:A:661:ASP:OD2	2.41	0.53
1:B:381:VAL:HG23	1:B:472:SER:HB3	1.89	0.53
1:B:816:TYR:CZ	1:B:931:ARG:HG3	2.44	0.53
1:A:696:MET:SD	1:A:704:PHE:HD1	2.31	0.53
1:A:825:ILE:HG12	1:A:927:LEU:HD23	1.91	0.53
1:B:669:PRO:HG2	1:B:697:HIS:HD2	1.71	0.53
1:A:665:VAL:HG11	1:A:677:SER:HA	1.90	0.52
1:B:969:TRP:CH2	1:B:975:LEU:HD13	2.44	0.52
1:B:222:VAL:HB	1:B:251:GLY:H	1.75	0.52
1:A:906:GLU:HG2	1:A:922:LEU:HD13	1.91	0.52
1:A:222:VAL:HB	1:A:251:GLY:H	1.74	0.52
1:A:892:GLU:OE2	1:A:895:ARG:NH1	2.43	0.52
1:B:340:TRP:HB3	1:B:364:TYR:CE1	2.45	0.52
1:A:290:HIS:HD1	1:A:465:TYR:HH	1.55	0.52
1:B:675:LYS:CG	1:B:722:GLN:HG3	2.40	0.52
1:B:504:LEU:HD12	1:B:898:LYS:HE3	1.92	0.52
1:B:582:VAL:HG12	1:B:583:ILE:H	1.73	0.52
1:B:582:VAL:HG12	1:B:583:ILE:N	2.25	0.51
1:B:351:LYS:NZ	1:B:372:VAL:HG11	2.26	0.51
1:B:906:GLU:HG2	1:B:922:LEU:HD13	1.92	0.51
1:B:361:VAL:HB	1:B:364:TYR:HB2	1.91	0.51
1:A:552:LYS:HG2	1:A:699:ILE:HD13	1.92	0.51
1:A:558:ARG:HG3	1:A:558:ARG:HH11	1.75	0.51
1:A:813:LEU:HD23	1:A:814:PRO:HD2	1.93	0.51
1:A:303:GLU:O	1:A:307:ILE:HG12	2.10	0.50
1:B:675:LYS:CB	1:B:722:GLN:HG3	2.41	0.50
1:A:731:TRP:HB3	1:A:1097:ILE:HG13	1.93	0.50
1:B:944:LYS:HE3	1:B:959:GLU:OE1	2.11	0.50
1:B:825:ILE:HG12	1:B:927:LEU:HD23	1.92	0.50
1:B:33:LEU:HD21	1:B:38:PRO:HG2	1.93	0.50
1:B:556:LEU:HD23	1:B:559:PHE:HZ	1.72	0.50
1:B:559:PHE:HB2	1:B:701:ARG:HG3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:LYS:CB	1:A:722:GLN:HG3	2.42	0.50
1:A:876:LYS:O	1:A:879:ILE:HG12	2.11	0.50
1:B:395:LEU:HD11	1:B:428:ALA:HA	1.94	0.50
1:B:431:HIS:CD2	1:B:440:LYS:HE2	2.47	0.49
1:A:361:VAL:HB	1:A:364:TYR:HB2	1.94	0.49
1:A:410:MET:HE2	1:A:440:LYS:HG3	1.94	0.49
1:B:307:ILE:HG22	1:B:522:VAL:HG21	1.94	0.49
1:A:1061:GLU:O	1:A:1065:THR:OG1	2.30	0.49
1:B:145:ALA:HB1	1:B:149:VAL:HG21	1.93	0.49
1:B:892:GLU:OE2	1:B:895:ARG:NH1	2.45	0.49
1:A:814:PRO:O	1:A:931:ARG:NH1	2.45	0.49
1:B:543:LEU:HD21	1:B:664:LEU:CD1	2.37	0.49
1:A:340:TRP:HB3	1:A:364:TYR:CE1	2.44	0.49
1:B:188:ASN:HB3	1:B:191:LYS:HD2	1.94	0.49
1:A:897:VAL:HG23	1:A:898:LYS:HG3	1.93	0.49
1:B:876:LYS:O	1:B:879:ILE:HG12	2.12	0.49
1:A:545:ILE:HD13	1:A:664:LEU:HB2	1.95	0.49
1:B:390:ARG:HG3	1:B:458:ILE:HG13	1.94	0.49
1:A:871:LEU:HA	1:A:874:ILE:HG22	1.95	0.49
1:A:596:VAL:HG12	1:A:598:LYS:H	1.78	0.48
1:B:943:LYS:HB2	1:B:965:LEU:CD1	2.42	0.48
1:B:620:ARG:HG3	1:B:627:GLN:HG2	1.95	0.48
1:B:731:TRP:HB3	1:B:1097:ILE:HG13	1.95	0.48
1:B:71:PHE:CD2	1:B:112:MET:HG2	2.48	0.48
1:B:479:VAL:HB	1:B:532:SER:HB3	1.94	0.48
1:B:871:LEU:HA	1:B:874:ILE:HG22	1.94	0.48
1:A:2:ALA:HB2	1:A:24:GLU:OE1	2.14	0.48
1:B:24:GLU:HA	1:B:685:LEU:HD23	1.96	0.48
1:B:543:LEU:O	1:B:583:ILE:HA	2.14	0.48
1:B:719:VAL:O	1:B:722:GLN:HB3	2.14	0.48
1:B:813:LEU:HD23	1:B:814:PRO:HD2	1.96	0.48
1:A:62:ASN:HA	1:A:65:GLU:OE2	2.13	0.47
1:A:675:LYS:CG	1:A:722:GLN:HG3	2.43	0.47
1:B:62:ASN:HA	1:B:65:GLU:OE2	2.14	0.47
1:B:897:VAL:HG23	1:B:898:LYS:HG3	1.96	0.47
1:A:744:PHE:HE1	1:A:1051:MET:HE2	1.80	0.47
1:B:1061:GLU:O	1:B:1065:THR:OG1	2.32	0.47
1:A:205:VAL:HG21	1:A:278:VAL:HG11	1.97	0.47
1:A:351:LYS:NZ	1:A:372:VAL:HG11	2.29	0.47
1:A:390:ARG:HG3	1:A:458:ILE:HG13	1.96	0.47
1:A:675:LYS:HB2	1:A:722:GLN:HG3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:PHE:CZ	1:B:137:THR:HG21	2.50	0.47
1:B:226:GLU:HA	1:B:229:ILE:HD12	1.96	0.47
1:B:803:LEU:HD11	1:B:945:GLN:NE2	2.29	0.47
1:A:188:ASN:HB3	1:A:191:LYS:HD2	1.95	0.47
1:A:226:GLU:HA	1:A:229:ILE:HD12	1.97	0.47
1:A:307:ILE:HG22	1:A:522:VAL:HG21	1.96	0.47
1:B:620:ARG:NH2	1:B:622:ARG:HA	2.30	0.47
1:B:803:LEU:HD13	1:B:947:VAL:HG13	1.97	0.47
1:B:22:ARG:HG2	1:B:27:LEU:HB2	1.96	0.47
1:B:566:ARG:HB2	1:B:573:VAL:HG13	1.96	0.47
1:B:571:ILE:HD12	1:B:586:THR:HG21	1.97	0.47
1:A:547:VAL:HG12	1:A:666:ALA:HB3	1.96	0.46
1:A:596:VAL:HG23	1:A:614:VAL:O	2.15	0.46
1:B:205:VAL:HG21	1:B:278:VAL:HG11	1.96	0.46
1:B:528:SER:HB2	1:B:531:ARG:NH2	2.30	0.46
1:B:410:MET:HE2	1:B:440:LYS:HG3	1.98	0.46
1:B:944:LYS:CB	1:B:961:ILE:HG23	2.45	0.46
1:A:71:PHE:CD2	1:A:112:MET:HG2	2.50	0.46
1:B:134:VAL:HG13	1:B:179:VAL:HG12	1.97	0.46
1:B:961:ILE:CD1	1:B:961:ILE:CB	2.83	0.46
1:B:433:THR:C	1:B:435:LYS:H	2.24	0.46
1:A:395:LEU:HD11	1:A:428:ALA:HA	1.97	0.46
1:A:696:MET:HG2	1:A:707:ALA:HB2	1.98	0.46
1:B:754:VAL:HG22	1:B:1069:THR:CG2	2.45	0.46
1:A:24:GLU:HA	1:A:685:LEU:HD23	1.98	0.46
1:A:237:LYS:HE2	1:B:637:VAL:CG1	2.46	0.46
1:A:958:ILE:HA	1:A:958:ILE:HD13	1.95	0.46
1:A:329:LEU:HD12	1:A:359:ILE:HD11	1.98	0.46
1:B:578:THR:HG21	1:B:583:ILE:HD13	1.96	0.45
1:B:797:VAL:HG23	1:B:987:LYS:HA	1.98	0.45
1:A:1002:PHE:HE1	1:A:1010:GLU:HG3	1.81	0.45
1:A:559:PHE:HB2	1:A:701:ARG:CZ	2.46	0.45
1:A:435:LYS:H	1:A:435:LYS:HD2	1.82	0.45
1:A:803:LEU:CD1	1:A:947:VAL:HG22	2.46	0.45
1:A:1003:THR:O	1:A:1007:ILE:HG13	2.15	0.45
1:B:803:LEU:CD1	1:B:947:VAL:HG22	2.46	0.45
1:B:956:MET:HE3	1:B:956:MET:HB3	1.72	0.45
1:B:997:HIS:CD2	1:B:997:HIS:N	2.85	0.45
1:B:1003:THR:O	1:B:1007:ILE:HG13	2.17	0.45
1:B:46:LEU:HD13	1:B:51:LEU:HD23	1.99	0.45
1:B:596:VAL:HG12	1:B:598:LYS:H	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:ALA:HB2	1:B:24:GLU:OE1	2.17	0.45
1:B:675:LYS:HB2	1:B:722:GLN:HG3	1.98	0.45
1:B:11:CYS:SG	1:B:29:CYS:HB3	2.57	0.45
1:B:620:ARG:O	1:B:644:ASP:N	2.47	0.45
1:A:616:ASN:ND2	1:A:629:THR:O	2.50	0.45
1:B:665:VAL:HG21	1:B:681:THR:HG23	1.97	0.44
1:B:558:ARG:HG3	1:B:558:ARG:HH11	1.82	0.44
1:A:958:ILE:CD1	1:A:958:ILE:CB	2.81	0.44
1:A:308:PHE:HE2	1:A:382:ILE:HD11	1.82	0.44
1:B:885:TRP:O	1:B:886:SER:HB2	2.18	0.44
1:A:33:LEU:HD12	1:A:48:ARG:HD2	2.00	0.44
1:A:566:ARG:HB2	1:A:573:VAL:HG13	1.98	0.44
1:A:668:ASP:HA	1:A:669:PRO:HD3	1.85	0.44
1:A:591:HIS:HB2	1:A:618:LEU:HD12	2.00	0.44
1:B:816:TYR:O	1:B:893:ALA:HB1	2.18	0.44
1:A:134:VAL:HG13	1:A:179:VAL:HG12	1.99	0.43
1:A:943:LYS:HB2	1:A:965:LEU:HD21	2.00	0.43
1:B:615:TYR:OH	1:B:723:ILE:HG12	2.17	0.43
1:B:543:LEU:HD12	1:B:662:GLU:HB3	1.99	0.43
1:B:814:PRO:O	1:B:931:ARG:NH1	2.51	0.43
1:A:128:PHE:CZ	1:A:137:THR:HG21	2.53	0.43
1:A:343:PHE:HB3	1:A:368:LEU:HD11	1.99	0.43
1:A:835:GLU:O	1:A:839:ILE:HG12	2.19	0.43
1:B:419:PRO:O	1:B:422:GLU:HB3	2.19	0.43
1:B:835:GLU:O	1:B:839:ILE:HG12	2.19	0.43
1:B:115:LEU:HD11	1:B:145:ALA:HB2	2.00	0.43
1:B:596:VAL:HG22	1:B:616:ASN:HB2	2.00	0.43
1:A:378:ILE:O	1:A:529:ARG:NH2	2.51	0.43
1:B:496:GLU:O	1:B:500:THR:HG23	2.18	0.43
1:A:715:ASP:OD1	1:A:718:LEU:HD13	2.19	0.43
1:B:189:ARG:HG3	1:B:217:THR:OG1	2.18	0.43
1:A:719:VAL:O	1:A:722:GLN:HB3	2.19	0.43
1:A:407:LEU:HD13	1:A:412:LEU:HD23	2.00	0.43
1:A:805:GLU:HG2	1:A:945:GLN:HB3	2.01	0.43
1:B:1077:ASP:HB3	1:B:1081:ARG:HH12	1.84	0.43
1:A:956:MET:HE3	1:A:956:MET:HB3	1.78	0.42
1:B:22:ARG:NE	1:B:28:PRO:O	2.52	0.42
1:B:622:ARG:HB2	1:B:642:ASN:OD1	2.20	0.42
1:B:942:VAL:HG22	1:B:963:GLU:O	2.19	0.42
1:A:996:LYS:HD3	1:A:996:LYS:HA	1.73	0.42
1:A:1077:ASP:HB3	1:A:1081:ARG:HH12	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:LYS:HG3	1:B:144:LEU:HG	2.02	0.42
1:A:189:ARG:HG3	1:A:217:THR:OG1	2.18	0.42
1:B:943:LYS:HE3	1:B:965:LEU:HD11	2.02	0.42
1:A:46:LEU:HD13	1:A:51:LEU:HD23	2.00	0.42
1:A:797:VAL:HG23	1:A:987:LYS:HA	2.02	0.42
1:A:805:GLU:CG	1:A:945:GLN:HB3	2.48	0.42
1:A:304:LEU:HD23	1:A:304:LEU:HA	1.79	0.42
1:A:301:LEU:HD23	1:A:325:LEU:HD11	2.01	0.42
1:A:665:VAL:HG21	1:A:681:THR:HG23	2.01	0.42
1:B:405:ARG:HD2	1:B:910:GLU:OE1	2.19	0.42
1:A:803:LEU:HD13	1:A:947:VAL:HG13	2.01	0.42
1:B:1097:ILE:HD13	1:B:1097:ILE:HA	1.99	0.42
1:A:405:ARG:HD2	1:A:910:GLU:OE1	2.20	0.42
1:B:436:GLU:O	1:B:440:LYS:HG2	2.20	0.42
1:A:154:PHE:CE1	1:A:163:LYS:HG3	2.55	0.41
1:A:430:GLU:O	1:A:431:HIS:C	2.63	0.41
1:A:816:TYR:O	1:A:893:ALA:HB1	2.20	0.41
1:A:436:GLU:O	1:A:440:LYS:HG2	2.20	0.41
1:A:737:SER:O	1:A:741:GLN:HG3	2.20	0.41
1:A:795:ASP:N	1:A:795:ASP:OD1	2.49	0.41
1:B:762:ILE:HG22	1:B:1045:PRO:HD3	2.01	0.41
1:A:379:LYS:HB3	1:A:525:VAL:HG11	2.02	0.41
1:A:758:VAL:O	1:A:761:TRP:HB2	2.20	0.41
1:B:610:LYS:HG2	1:B:1087:GLN:HG2	2.02	0.41
1:A:155:TYR:CE2	1:A:158:MET:HE2	2.55	0.41
1:A:824:GLU:OE2	1:A:931:ARG:NH2	2.52	0.41
1:B:175:TYR:HB2	1:B:178:LEU:HD21	2.03	0.41
1:B:545:ILE:HD13	1:B:585:PHE:HB3	2.03	0.41
1:B:715:ASP:OD1	1:B:718:LEU:HD13	2.20	0.41
1:B:1040:TYR:HB2	1:B:1042:ARG:HD2	2.02	0.41
1:A:958:ILE:CD1	1:A:958:ILE:CA	2.95	0.41
1:A:5:SER:HB3	1:A:613:PRO:HD2	2.03	0.41
1:A:1002:PHE:HD1	1:A:1006:SER:OG	2.04	0.41
1:B:5:SER:HB3	1:B:613:PRO:HD2	2.02	0.41
1:B:351:LYS:HZ2	1:B:372:VAL:HG11	1.86	0.41
1:B:543:LEU:HD23	1:B:545:ILE:HG13	2.03	0.41
1:B:737:SER:O	1:B:741:GLN:HG3	2.20	0.41
1:B:795:ASP:OD1	1:B:795:ASP:N	2.51	0.41
1:B:388:SER:HA	1:B:461:ASP:H	1.86	0.41
1:B:545:ILE:O	1:B:585:PHE:HA	2.21	0.41
1:B:551:THR:O	1:B:552:LYS:C	2.64	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:596:VAL:HG23	1:B:614:VAL:O	2.21	0.41
1:B:124:SER:HB3	1:B:199:PHE:HD2	1.86	0.40
1:A:696:MET:HG2	1:A:707:ALA:CB	2.51	0.40
1:A:1040:TYR:HB2	1:A:1042:ARG:HD2	2.03	0.40
1:B:379:LYS:HB3	1:B:525:VAL:HG11	2.04	0.40
1:B:541:ARG:O	1:B:581:GLY:HA3	2.22	0.40
1:B:438:VAL:HG21	1:B:455:LEU:HD22	2.02	0.40
1:A:685:LEU:HD12	1:A:685:LEU:HA	1.79	0.40
1:B:593:TYR:HD1	1:B:679:ASP:HB3	1.87	0.40
1:A:551:THR:O	1:A:555:THR:HG23	2.21	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	
1	A	1100/1104 (100%)	997 (91%)	95 (9%)	8 (1%)	18	51
1	B	1100/1104 (100%)	988 (90%)	99 (9%)	13 (1%)	10	41
All	All	2200/2208 (100%)	1985 (90%)	194 (9%)	21 (1%)	12	44

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	417	GLU
1	A	792	LYS
1	A	791	GLY
1	B	39	SER
1	B	562	ARG
1	B	791	GLY
1	B	792	LYS
1	A	415	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	30	GLU
1	B	173	ASP
1	B	415	ALA
1	B	432	LEU
1	B	538	ASP
1	B	886	SER
1	B	983	HIS
1	A	173	ASP
1	A	431	HIS
1	A	983	HIS
1	A	76	GLY
1	B	76	GLY
1	B	598	LYS

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	
1	A	992/993 (100%)	914 (92%)	78 (8%)	11	37
1	B	992/993 (100%)	879 (89%)	113 (11%)	5	25
All	All	1984/1986 (100%)	1793 (90%)	191 (10%)	8	31

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLU
1	A	55	ARG
1	A	65	GLU
1	A	66	ASP
1	A	73	LYS
1	A	80	THR
1	A	90	ILE
1	A	113	THR
1	A	115	LEU
1	A	120	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	146	ASP
1	A	165	LYS
1	A	208	VAL
1	A	241	ILE
1	A	261	LYS
1	A	280	ARG
1	A	281	LEU
1	A	284	VAL
1	A	299	GLU
1	A	321	GLU
1	A	343	PHE
1	A	345	LYS
1	A	358	LEU
1	A	364	TYR
1	A	376	GLU
1	A	390	ARG
1	A	396	ASP
1	A	400	ARG
1	A	410	MET
1	A	432	LEU
1	A	435	LYS
1	A	436	GLU
1	A	439	GLU
1	A	454	ASP
1	A	456	GLU
1	A	537	THR
1	A	539	THR
1	A	545	ILE
1	A	555	THR
1	A	564	SER
1	A	573	VAL
1	A	619	LYS
1	A	647	THR
1	A	685	LEU
1	A	709	GLU
1	A	722	GLN
1	A	725	ARG
1	A	743	ARG
1	A	774	LYS
1	A	775	ASP
1	A	786	ASN
1	A	793	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	797	VAL
1	A	805	GLU
1	A	813	LEU
1	A	819	SER
1	A	820	SER
1	A	828	LYS
1	A	843	LEU
1	A	878	ASP
1	A	881	MET
1	A	913	LEU
1	A	927	LEU
1	A	931	ARG
1	A	942	VAL
1	A	956	MET
1	A	958	ILE
1	A	961	ILE
1	A	965	LEU
1	A	966	ARG
1	A	978	SER
1	A	995	LYS
1	A	997	HIS
1	A	1035	VAL
1	A	1067	GLU
1	A	1077	ASP
1	A	1078	LYS
1	A	1101	MET
1	B	9	HIS
1	B	21	GLU
1	B	29	CYS
1	B	30	GLU
1	B	35	GLU
1	B	55	ARG
1	B	65	GLU
1	B	66	ASP
1	B	73	LYS
1	B	80	THR
1	B	90	ILE
1	B	102	THR
1	B	113	THR
1	B	115	LEU
1	B	120	LYS
1	B	124	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	146	ASP
1	B	149	VAL
1	B	170	PHE
1	B	187	LYS
1	B	208	VAL
1	B	241	ILE
1	B	261	LYS
1	B	280	ARG
1	B	281	LEU
1	B	284	VAL
1	B	299	GLU
1	B	321	GLU
1	B	343	PHE
1	B	358	LEU
1	B	364	TYR
1	B	376	GLU
1	B	390	ARG
1	B	396	ASP
1	B	400	ARG
1	B	410	MET
1	B	412	LEU
1	B	416	GLN
1	B	418	ASN
1	B	429	LYS
1	B	430	GLU
1	B	432	LEU
1	B	433	THR
1	B	435	LYS
1	B	436	GLU
1	B	439	GLU
1	B	454	ASP
1	B	456	GLU
1	B	476	LEU
1	B	492	GLU
1	B	496	GLU
1	B	528	SER
1	B	542	SER
1	B	543	LEU
1	B	545	ILE
1	B	547	VAL
1	B	554	GLU
1	B	555	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	564	SER
1	B	573	VAL
1	B	583	ILE
1	B	586	THR
1	B	619	LYS
1	B	629	THR
1	B	640	SER
1	B	647	THR
1	B	661	ASP
1	B	682	GLN
1	B	685	LEU
1	B	695	GLU
1	B	696	MET
1	B	702	TYR
1	B	709	GLU
1	B	722	GLN
1	B	725	ARG
1	B	743	ARG
1	B	764	GLU
1	B	774	LYS
1	B	775	ASP
1	B	786	ASN
1	B	793	ILE
1	B	797	VAL
1	B	805	GLU
1	B	813	LEU
1	B	819	SER
1	B	820	SER
1	B	828	LYS
1	B	843	LEU
1	B	845	GLU
1	B	878	ASP
1	B	881	MET
1	B	927	LEU
1	B	931	ARG
1	B	942	VAL
1	B	944	LYS
1	B	956	MET
1	B	958	ILE
1	B	960	GLN
1	B	961	ILE
1	B	963	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	965	LEU
1	B	966	ARG
1	B	977	VAL
1	B	995	LYS
1	B	996	LYS
1	B	997	HIS
1	B	1035	VAL
1	B	1052	VAL
1	B	1067	GLU
1	B	1077	ASP
1	B	1087	GLN
1	B	1097	ILE
1	B	1101	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	23	ASN
1	A	142	GLN
1	A	317	GLN
1	A	335	ASN
1	A	346	ASN
1	A	431	HIS
1	A	477	ASN
1	A	682	GLN
1	A	722	GLN
1	A	804	GLN
1	A	834	GLN
1	A	865	ASN
1	B	8	HIS
1	B	23	ASN
1	B	317	GLN
1	B	335	ASN
1	B	346	ASN
1	B	431	HIS
1	B	477	ASN
1	B	682	GLN
1	B	722	GLN
1	B	804	GLN
1	B	834	GLN
1	B	865	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	970	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	1102/1104 (99%)	0.56	57 (5%)	33 20	48, 100, 169, 216	0
1	B	1102/1104 (99%)	0.43	37 (3%)	48 29	25, 90, 175, 224	0
All	All	2204/2208 (99%)	0.49	94 (4%)	40 23	25, 96, 174, 224	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	594	ASP	4.8
1	B	15	GLY	4.3
1	A	896	PRO	4.1
1	A	748	ASN	4.1
1	A	851	TYR	3.9
1	A	671	VAL	3.9
1	B	57	TYR	3.8
1	A	282	VAL	3.5
1	B	374	LEU	3.5
1	B	896	PRO	3.4
1	B	278	VAL	3.4
1	B	395	LEU	3.3
1	A	595	LEU	3.3
1	A	39	SER	3.2
1	B	39	SER	3.2
1	B	594	ASP	3.2
1	A	38	PRO	3.2
1	B	1063	TYR	3.2
1	A	217	THR	3.1
1	A	1008	VAL	3.1
1	A	719	VAL	3.0
1	B	421	VAL	3.0
1	A	57	TYR	2.9
1	A	374	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	15	GLY	2.8
1	A	518	TRP	2.8
1	A	12	ILE	2.7
1	A	663	ILE	2.7
1	A	109	PHE	2.7
1	B	574	HIS	2.7
1	B	568	GLU	2.6
1	A	750	SER	2.6
1	A	818	THR	2.6
1	A	424	LEU	2.5
1	A	278	VAL	2.5
1	A	668	ASP	2.5
1	A	560	LEU	2.5
1	A	747	SER	2.5
1	A	722	GLN	2.5
1	A	785	VAL	2.4
1	A	672	GLU	2.4
1	B	424	LEU	2.4
1	A	761	TRP	2.4
1	A	659	GLU	2.4
1	B	575	GLU	2.4
1	B	887	THR	2.4
1	B	593	TYR	2.4
1	A	880	PHE	2.3
1	A	219	LEU	2.3
1	B	880	PHE	2.3
1	B	518	TRP	2.3
1	A	578	THR	2.3
1	A	667	THR	2.3
1	A	582	VAL	2.3
1	B	205	VAL	2.3
1	A	526	GLU	2.2
1	B	423	GLU	2.2
1	B	824	GLU	2.2
1	B	665	VAL	2.2
1	B	273	LEU	2.2
1	A	193	SER	2.2
1	A	938	ALA	2.2
1	B	192	LEU	2.2
1	A	596	VAL	2.2
1	B	752	GLY	2.2
1	A	755	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	55	ARG	2.1
1	B	515	GLU	2.1
1	A	239	GLY	2.1
1	B	26	GLY	2.1
1	B	878	ASP	2.1
1	A	864	GLN	2.1
1	A	41	ILE	2.1
1	A	583	ILE	2.1
1	B	218	LEU	2.1
1	A	741	GLN	2.1
1	B	939	ALA	2.1
1	B	279	GLY	2.1
1	B	361	VAL	2.1
1	B	818	THR	2.1
1	A	262	PRO	2.1
1	B	815	PRO	2.1
1	A	412	LEU	2.1
1	A	891	HIS	2.1
1	A	688	THR	2.1
1	B	996	LYS	2.0
1	B	946	ILE	2.0
1	A	64	TYR	2.0
1	A	343	PHE	2.0
1	A	401	PHE	2.0
1	A	1043	VAL	2.0
1	A	144	LEU	2.0
1	B	392	SER	2.0
1	A	61	TRP	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](#)

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, 95th 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($\text{\AA}^2$)	Q<0.9
2	ZN	A	2001	1/1	0.98	0.05	137,137,137,137	0
2	ZN	B	2001	1/1	0.98	0.05	137,137,137,137	0
2	ZN	A	2002	1/1	0.99	0.04	75,75,75,75	0
2	ZN	B	2002	1/1	0.99	0.03	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.