



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:21 PM UTC

PDB ID : 6AES / pdb_00006aes
Title : Crystal structure of Nucleoside diphosphate kinase from *Pseudomonas aeruginosa* at 3.55 Å resolution.
Authors : Sikarwar, J.; Singh, P.K.; Sharma, S.; Singh, T.P.
Deposited on : 2018-08-06
Resolution : 3.55 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

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Mol	Chain	Length	Quality of chain
1	F	143	% 73% 17% 8% •
1	G	143	3% 75% 19% 6% •
1	H	143	% 76% 21% ••

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8759 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 Nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	143	Total	C	N	O	S	0	0	0
			1094	687	192	210	5			
1	B	143	Total	C	N	O	S	0	0	0
			1094	687	192	210	5			
1	C	143	Total	C	N	O	S	0	0	0
			1094	687	192	210	5			
1	D	143	Total	C	N	O	S	0	0	0
			1094	687	192	210	5			
1	E	143	Total	C	N	O	S	0	0	0
			1094	687	192	210	5			
1	F	143	Total	C	N	O	S	0	0	0
			1094	687	192	210	5			
1	G	143	Total	C	N	O	S	0	0	0
			1094	687	192	210	5			
1	H	143	Total	C	N	O	S	0	0	0
			1094	687	192	210	5			

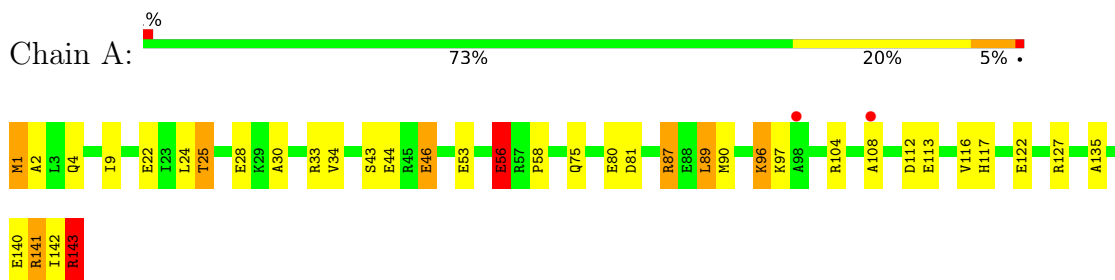
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	O	0	0
			1	1		
2	E	4	Total	O	0	0
			4	4		
2	F	1	Total	O	0	0
			1	1		
2	G	1	Total	O	0	0
			1	1		

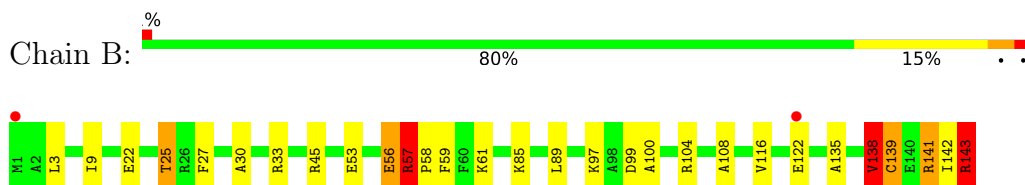
3 Residue-property plots

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.

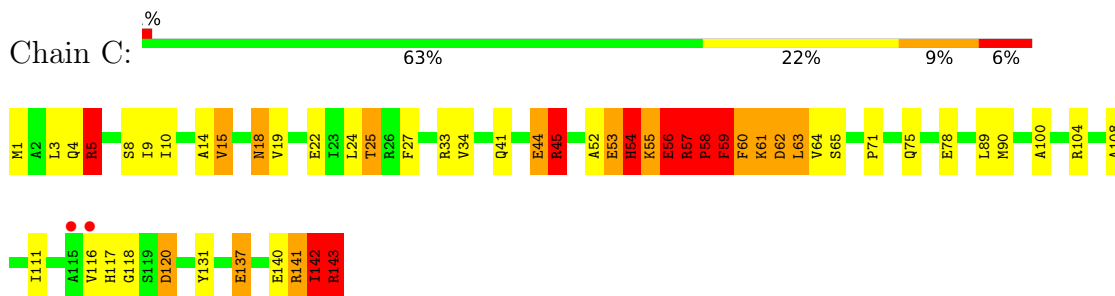
- Molecule 1: Nucleoside diphosphate kinase



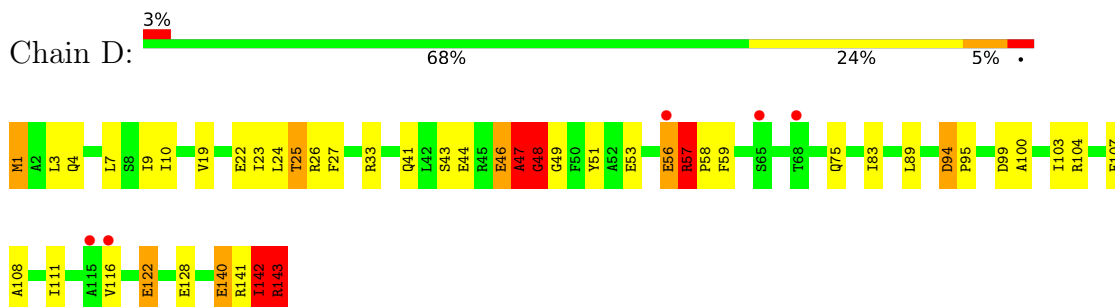
- Molecule 1: Nucleoside diphosphate kinase



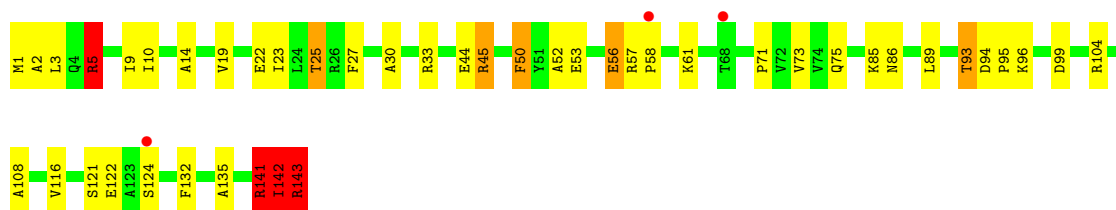
- Molecule 1: Nucleoside diphosphate kinase



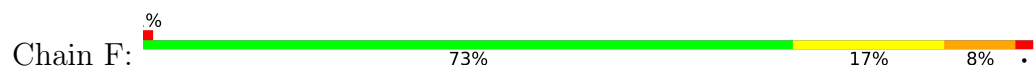
- Molecule 1: Nucleoside diphosphate kinase



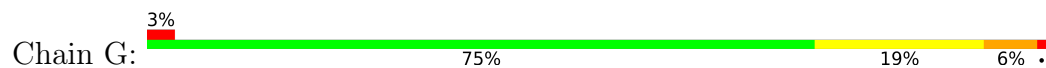
● Molecule 1: Nucleoside diphosphate kinase



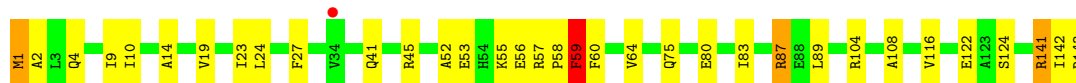
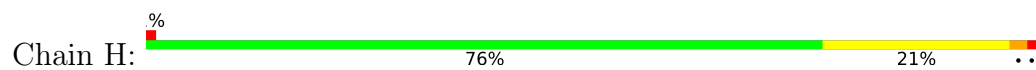
● Molecule 1: Nucleoside diphosphate kinase



● Molecule 1: Nucleoside diphosphate kinase



● Molecule 1: Nucleoside diphosphate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	68.57Å 70.88Å 71.10Å 99.60° 109.12° 90.25°	Depositor
Resolution (Å)	45.98 – 3.55 45.98 – 3.55	Depositor EDS
% Data completeness (in resolution range)	98.6 (45.98-3.55) 98.6 (45.98-3.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.286 , 0.332 0.287 , 0.330	Depositor DCC
R_{free} test set	741 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	111.1	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 109.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	8759	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.09% 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	A	0.81	0/1109	1.30	7/1492 (0.5%)
1	B	0.76	1/1109 (0.1%)	1.17	4/1492 (0.3%)
1	C	1.29	9/1109 (0.8%)	1.49	19/1492 (1.3%)
1	D	0.84	2/1109 (0.2%)	1.32	10/1492 (0.7%)
1	E	1.00	6/1109 (0.5%)	1.37	8/1492 (0.5%)
1	F	0.97	3/1109 (0.3%)	1.31	9/1492 (0.6%)
1	G	0.78	1/1109 (0.1%)	1.20	2/1492 (0.1%)
1	H	0.82	1/1109 (0.1%)	1.27	6/1492 (0.4%)
All	All	0.92	23/8872 (0.3%)	1.31	65/11936 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
1	C	0	7
1	D	0	5
1	E	0	5
1	F	0	2
1	G	0	4
1	H	0	2
All	All	0	33

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	60	PHE	N-CA	-18.19	1.22	1.46
1	E	143	ARG	CZ-NH1	11.81	1.49	1.32
1	C	56	GLU	N-CA	-11.23	1.31	1.46
1	F	81	ASP	C-O	-10.83	1.10	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	143	ARG	NE-CZ	9.50	1.43	1.33
1	E	5	ARG	CZ-NH2	9.26	1.45	1.33
1	H	60	PHE	N-CA	-9.23	1.35	1.46
1	F	83	ILE	C-O	-8.90	1.13	1.24
1	E	143	ARG	CD-NE	8.78	1.58	1.46
1	C	53	GLU	C-O	-8.69	1.12	1.24
1	C	59	PHE	N-CA	-8.09	1.35	1.46
1	C	54	HIS	ND1-CE1	8.03	1.40	1.32
1	C	100	ALA	C-O	-7.93	1.14	1.24
1	C	56	GLU	C-O	-7.64	1.14	1.24
1	C	61	LYS	N-CA	-7.33	1.35	1.46
1	D	48	GLY	N-CA	-7.17	1.35	1.45
1	F	80	GLU	N-CA	6.94	1.54	1.45
1	B	61	LYS	N-CA	-6.00	1.39	1.46
1	E	143	ARG	CZ-NH2	5.93	1.41	1.33
1	D	47	ALA	C-N	-5.81	1.25	1.33
1	C	60	PHE	C-O	-5.59	1.17	1.24
1	E	142	ILE	C-O	-5.45	1.17	1.23
1	G	46	GLU	CD-OE1	-5.16	1.15	1.25

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	143	ARG	NE-CZ-NH2	15.19	132.87	119.20
1	E	143	ARG	NH1-CZ-NH2	-14.78	100.09	119.30
1	C	59	PHE	CA-CB-CG	-12.26	101.54	113.80
1	C	58	PRO	CA-N-CD	-10.55	97.23	112.00
1	E	143	ARG	CD-NE-CZ	10.48	139.08	124.40
1	H	59	PHE	CB-CA-C	-10.14	95.26	111.28
1	D	47	ALA	CA-C-N	-9.88	103.39	121.07
1	D	47	ALA	C-N-CA	-9.88	103.39	121.07
1	C	53	GLU	CB-CA-C	-9.01	90.48	110.21
1	A	96	LYS	CB-CA-C	-7.87	98.22	110.81
1	B	56	GLU	CB-CA-C	-7.82	96.04	109.65
1	F	139	CYS	CA-C-N	7.61	131.93	121.05
1	F	139	CYS	C-N-CA	7.61	131.93	121.05
1	C	58	PRO	N-CA-C	-7.30	97.42	112.47
1	D	94	ASP	CB-CA-C	-7.29	97.84	109.51
1	E	143	ARG	N-CA-CB	-7.26	98.16	110.50
1	H	87	ARG	CG-CD-NE	-7.21	96.14	112.00
1	A	1	MET	CB-CA-C	-7.17	96.48	110.10
1	C	44	GLU	CB-CA-C	-7.12	99.41	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	80	GLU	CB-CG-CD	7.07	124.62	112.60
1	B	122	GLU	CB-CG-CD	-6.83	100.98	112.60
1	F	83	ILE	O-C-N	-6.58	114.35	122.57
1	A	122	GLU	CB-CA-C	-6.49	100.02	110.79
1	D	57	ARG	CG-CD-NE	-6.48	97.74	112.00
1	G	56	GLU	N-CA-CB	-6.48	100.33	110.44
1	D	122	GLU	CB-CA-C	-6.24	100.44	110.79
1	F	94	ASP	CB-CA-C	6.22	118.34	109.38
1	E	94	ASP	CB-CA-C	-6.21	99.57	109.51
1	C	54	HIS	CA-C-N	-6.20	107.81	122.20
1	C	54	HIS	C-N-CA	-6.20	107.81	122.20
1	C	58	PRO	CB-CA-C	6.17	121.75	111.56
1	B	57	ARG	CG-CD-NE	-6.13	98.51	112.00
1	F	56	GLU	CB-CA-C	-6.09	99.92	110.09
1	D	47	ALA	CB-CA-C	-6.02	98.43	110.42
1	H	52	ALA	CA-C-N	6.00	129.81	120.82
1	H	52	ALA	C-N-CA	6.00	129.81	120.82
1	A	56	GLU	CB-CA-C	-5.99	100.09	110.09
1	D	56	GLU	CB-CA-C	-5.95	98.31	109.72
1	D	49	GLY	CA-C-N	5.94	128.16	120.44
1	D	49	GLY	C-N-CA	5.94	128.16	120.44
1	C	140	GLU	CB-CG-CD	-5.86	102.63	112.60
1	A	1	MET	CA-C-N	-5.86	110.36	121.54
1	A	1	MET	C-N-CA	-5.86	110.36	121.54
1	C	61	LYS	N-CA-CB	-5.75	103.73	112.47
1	C	58	PRO	CA-C-N	5.70	132.42	121.54
1	C	58	PRO	C-N-CA	5.70	132.42	121.54
1	E	45	ARG	NE-CZ-NH1	-5.62	115.89	121.50
1	F	4	GLN	CB-CG-CD	-5.60	103.08	112.60
1	C	61	LYS	CA-C-O	-5.58	113.88	120.57
1	C	137	GLU	CB-CA-C	-5.56	101.57	110.79
1	F	140	GLU	CB-CG-CD	-5.53	103.20	112.60
1	C	44	GLU	CB-CG-CD	-5.46	103.33	112.60
1	C	54	HIS	ND1-CE1-NE2	-5.46	102.94	108.40
1	B	138	VAL	N-CA-CB	5.32	116.86	110.31
1	D	140	GLU	N-CA-CB	5.31	117.77	109.97
1	F	137	GLU	CB-CA-C	-5.28	100.54	110.67
1	H	53	GLU	N-CA-CB	-5.26	101.21	109.78
1	G	56	GLU	CB-CG-CD	-5.21	103.73	112.60
1	C	120	ASP	CA-CB-CG	5.17	117.77	112.60
1	E	142	ILE	N-CA-C	-5.17	102.32	109.46
1	A	89	LEU	CB-CA-C	-5.16	100.77	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	60	PHE	N-CA-CB	-5.13	102.58	110.12
1	C	15	VAL	CA-C-N	5.05	127.56	120.28
1	C	15	VAL	C-N-CA	5.05	127.56	120.28
1	E	93	THR	OG1-CB-CG2	-5.01	99.28	109.30

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	ARG	Sidechain
1	A	143	ARG	Sidechain
1	A	33	ARG	Sidechain
1	A	87	ARG	Sidechain
1	B	141	ARG	Sidechain
1	B	143	ARG	Sidechain
1	B	33	ARG	Sidechain
1	B	45	ARG	Sidechain
1	C	141	ARG	Sidechain
1	C	143	ARG	Sidechain
1	C	33	ARG	Sidechain
1	C	45	ARG	Sidechain
1	C	5	ARG	Sidechain
1	C	54	HIS	Peptide
1	C	57	ARG	Sidechain
1	D	141	ARG	Sidechain
1	D	143	ARG	Sidechain
1	D	33	ARG	Sidechain
1	D	46	GLU	Peptide
1	D	48	GLY	Peptide
1	E	141	ARG	Sidechain
1	E	142	ILE	Peptide
1	E	143	ARG	Sidechain
1	E	5	ARG	Sidechain
1	E	57	ARG	Sidechain
1	F	143	ARG	Sidechain
1	F	33	ARG	Sidechain
1	G	141	ARG	Sidechain
1	G	143	ARG	Sidechain
1	G	33	ARG	Sidechain
1	G	57	ARG	Sidechain
1	H	141	ARG	Sidechain
1	H	45	ARG	Sidechain

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	1094	0	1103	30	3
1	B	1094	0	1103	32	2
1	C	1094	0	1103	84	1
1	D	1094	0	1103	41	2
1	E	1094	0	1103	42	2
1	F	1094	0	1103	36	3
1	G	1094	0	1103	26	3
1	H	1094	0	1103	34	0
2	B	1	0	0	0	0
2	E	4	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
All	All	8759	0	8824	285	8

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 16.

All (285) 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:D:44:GLU:O	1:D:47:ALA:HB2	1.16	1.29
1:C:57:ARG:HH12	1:H:58:PRO:HB3	1.12	1.14
1:F:4:GLN:OE1	1:F:83:ILE:HB	1.49	1.12
1:C:62:ASP:O	1:C:65:SER:N	1.83	1.11
1:C:62:ASP:O	1:C:64:VAL:N	1.85	1.10
1:D:44:GLU:O	1:D:47:ALA:CB	2.00	1.09
1:C:62:ASP:O	1:C:63:LEU:C	1.91	1.08
1:C:57:ARG:NH2	1:H:58:PRO:HA	1.68	1.07
1:A:1:MET:O	1:A:2:ALA:HB3	1.51	1.04
1:D:142:ILE:O	1:D:143:ARG:O	1.76	1.03
1:C:57:ARG:NH1	1:H:58:PRO:HB3	1.75	1.02
1:C:56:GLU:OE1	1:H:56:GLU:HB2	1.57	1.02
1:C:62:ASP:HA	1:C:65:SER:HB3	1.40	1.01
1:D:19:VAL:HG11	1:D:107:PHE:CD1	1.97	1.00
1:F:83:ILE:HG23	1:F:83:ILE:O	1.63	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:CYS:SG	1:C:71:PRO:HG3	2.04	0.98
1:C:57:ARG:HH22	1:H:58:PRO:HA	1.18	0.96
1:C:57:ARG:NH1	1:H:58:PRO:CB	2.28	0.96
1:F:83:ILE:O	1:F:84:ALA:HB3	1.65	0.96
1:C:142:ILE:HD12	1:C:142:ILE:H	1.32	0.95
1:A:1:MET:O	1:A:2:ALA:CB	2.09	0.94
1:C:45:ARG:HG3	1:C:45:ARG:HH11	1.33	0.93
1:D:19:VAL:HG11	1:D:107:PHE:CE1	2.04	0.92
1:D:143:ARG:CZ	1:E:122:GLU:OE2	2.19	0.90
1:D:24:LEU:HD21	1:D:75:GLN:NE2	1.86	0.90
1:F:10:ILE:HG22	1:F:73:VAL:HB	1.52	0.90
1:C:62:ASP:HA	1:C:65:SER:CB	2.01	0.90
1:C:58:PRO:HA	1:C:59:PHE:CE1	2.07	0.89
1:C:57:ARG:HH12	1:H:58:PRO:CB	1.85	0.89
1:C:56:GLU:CD	1:H:56:GLU:HB2	1.97	0.88
1:F:83:ILE:O	1:F:84:ALA:CB	2.15	0.88
1:A:58:PRO:HB2	1:E:53:GLU:HA	1.57	0.86
1:F:80:GLU:O	1:F:81:ASP:OD1	1.94	0.84
1:D:19:VAL:CG1	1:D:107:PHE:CE1	2.61	0.84
1:G:45:ARG:HG3	1:G:45:ARG:HH11	1.41	0.83
1:C:55:LYS:HG2	1:C:55:LYS:O	1.75	0.83
1:D:43:SER:HB3	1:D:46:GLU:HG3	1.60	0.83
1:B:139:CYS:SG	1:C:71:PRO:CG	2.67	0.83
1:C:58:PRO:HA	1:C:59:PHE:CD1	2.13	0.82
1:A:30:ALA:HB2	1:A:89:LEU:HD21	1.61	0.82
1:C:9:ILE:O	1:C:116:VAL:HG13	1.81	0.79
1:C:57:ARG:HG3	1:C:58:PRO:HD3	1.65	0.79
1:C:60:PHE:HB2	1:C:62:ASP:OD2	1.82	0.79
1:C:57:ARG:NH1	1:H:58:PRO:HG3	1.98	0.79
1:C:34:VAL:O	1:C:141:ARG:NH1	2.15	0.79
1:E:71:PRO:HB3	1:F:139:CYS:SG	2.23	0.78
1:B:57:ARG:HG3	1:B:58:PRO:HD2	1.64	0.78
1:F:83:ILE:O	1:F:83:ILE:CG2	2.31	0.78
1:F:10:ILE:HD11	1:F:23:ILE:HD12	1.65	0.77
1:C:62:ASP:O	1:C:64:VAL:C	2.28	0.77
1:C:57:ARG:HB3	1:C:58:PRO:CD	2.15	0.76
1:C:58:PRO:O	1:C:59:PHE:O	2.04	0.76
1:F:94:ASP:HB2	1:F:111:ILE:CD1	2.17	0.75
1:F:10:ILE:CG2	1:F:73:VAL:HB	2.17	0.74
1:C:57:ARG:NH1	1:H:58:PRO:CG	2.50	0.74
1:D:48:GLY:HA2	1:D:51:TYR:H	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:ARG:CG	1:C:58:PRO:HD3	2.18	0.74
1:C:60:PHE:O	1:C:61:LYS:HB2	1.90	0.71
1:A:43:SER:H	1:A:46:GLU:HG3	1.56	0.71
1:E:141:ARG:HH21	1:E:141:ARG:HG3	1.57	0.70
1:D:94:ASP:OD1	1:D:111:ILE:HD12	1.91	0.69
1:F:143:ARG:HG3	1:F:143:ARG:HH11	1.55	0.69
1:G:45:ARG:HH11	1:G:45:ARG:CG	2.06	0.69
1:C:57:ARG:NH2	1:H:58:PRO:CA	2.54	0.68
1:D:24:LEU:HD21	1:D:75:GLN:HE22	1.58	0.68
1:C:142:ILE:HD12	1:C:142:ILE:N	2.01	0.67
1:E:1:MET:HG3	1:E:2:ALA:H	1.59	0.67
1:C:62:ASP:C	1:C:64:VAL:N	2.53	0.67
1:B:57:ARG:HG2	1:B:59:PHE:CE2	2.30	0.66
1:E:143:ARG:O	1:E:143:ARG:HG2	1.94	0.66
1:C:56:GLU:OE1	1:H:56:GLU:CB	2.41	0.65
1:C:142:ILE:O	1:C:143:ARG:C	2.40	0.65
1:C:59:PHE:CD1	1:C:59:PHE:N	2.56	0.65
1:B:143:ARG:HG3	1:B:143:ARG:NH1	2.12	0.65
1:G:59:PHE:O	1:G:61:LYS:N	2.29	0.65
1:G:59:PHE:HD1	1:G:60:PHE:N	1.93	0.65
1:C:62:ASP:CA	1:C:65:SER:HB3	2.24	0.64
1:E:50:PHE:CE2	1:E:132:PHE:HE2	2.15	0.64
1:E:50:PHE:CD2	1:E:132:PHE:CE2	2.88	0.62
1:C:62:ASP:O	1:C:64:VAL:CA	2.48	0.62
1:H:83:ILE:HD11	1:H:122:GLU:HA	1.80	0.62
1:C:57:ARG:CZ	1:H:58:PRO:HA	2.30	0.61
1:H:57:ARG:HD2	1:H:58:PRO:HD3	1.82	0.61
1:A:24:LEU:O	1:A:28:GLU:HG3	2.00	0.61
1:A:113:GLU:OE1	1:E:122:GLU:OE1	2.17	0.61
1:D:143:ARG:NH1	1:E:122:GLU:OE2	2.35	0.60
1:D:142:ILE:O	1:D:143:ARG:C	2.45	0.59
1:B:141:ARG:NH1	1:C:15:VAL:CG1	2.66	0.59
1:F:77:LEU:HD12	1:F:86:ASN:ND2	2.16	0.59
1:G:90:MET:HE1	1:G:116:VAL:HB	1.85	0.59
1:C:55:LYS:O	1:C:55:LYS:CG	2.42	0.59
1:C:57:ARG:CB	1:C:58:PRO:CD	2.79	0.59
1:C:58:PRO:CA	1:C:59:PHE:CD1	2.85	0.58
1:B:141:ARG:HH11	1:C:15:VAL:HG12	1.67	0.58
1:D:24:LEU:HD21	1:D:75:GLN:CD	2.28	0.58
1:F:94:ASP:HB2	1:F:111:ILE:HD13	1.86	0.58
1:D:94:ASP:OD1	1:D:111:ILE:CD1	2.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:PHE:CD1	1:E:50:PHE:C	2.81	0.57
1:E:142:ILE:C	1:E:142:ILE:HD12	2.29	0.57
1:E:50:PHE:HD2	1:E:132:PHE:CE2	2.22	0.57
1:H:24:LEU:HD21	1:H:75:GLN:OE1	2.04	0.57
1:C:57:ARG:CZ	1:H:58:PRO:CA	2.83	0.57
1:D:142:ILE:HG22	1:D:143:ARG:N	2.20	0.56
1:F:27:PHE:CD1	1:F:89:LEU:HD11	2.41	0.56
1:A:58:PRO:HB2	1:E:53:GLU:CA	2.33	0.56
1:B:141:ARG:HH11	1:C:15:VAL:CG1	2.19	0.56
1:G:59:PHE:CD1	1:G:60:PHE:N	2.74	0.56
1:E:73:VAL:HG12	1:E:75:GLN:HE21	1.72	0.55
1:C:24:LEU:HD21	1:C:75:GLN:OE1	2.05	0.55
1:F:89:LEU:C	1:F:89:LEU:HD12	2.32	0.55
1:C:57:ARG:CB	1:C:58:PRO:HD3	2.37	0.55
1:A:142:ILE:HG22	1:A:143:ARG:N	2.22	0.55
1:E:50:PHE:CD2	1:E:132:PHE:HE2	2.24	0.55
1:C:56:GLU:OE2	1:H:56:GLU:HB2	2.07	0.54
1:B:141:ARG:NH1	1:C:15:VAL:HG12	2.22	0.54
1:C:89:LEU:C	1:C:89:LEU:HD12	2.33	0.54
1:F:3:LEU:HD12	1:F:3:LEU:H	1.73	0.54
1:G:27:PHE:CD1	1:G:89:LEU:HD11	2.43	0.54
1:B:89:LEU:HD12	1:B:89:LEU:C	2.32	0.54
1:G:77:LEU:HD12	1:G:86:ASN:OD1	2.07	0.54
1:C:3:LEU:HD12	1:C:3:LEU:N	2.22	0.54
1:H:1:MET:O	1:H:80:GLU:OE1	2.25	0.54
1:H:9:ILE:O	1:H:116:VAL:HG13	2.08	0.54
1:D:3:LEU:HD12	1:D:3:LEU:O	2.08	0.54
1:D:89:LEU:C	1:D:89:LEU:HD12	2.34	0.53
1:B:27:PHE:CD1	1:B:89:LEU:HD11	2.44	0.53
1:B:143:ARG:NH1	1:B:143:ARG:CG	2.71	0.53
1:C:62:ASP:HA	1:C:65:SER:HB2	1.90	0.53
1:C:18:ASN:N	1:C:18:ASN:HD22	2.06	0.53
1:E:89:LEU:HD12	1:E:89:LEU:C	2.33	0.53
1:H:83:ILE:CD1	1:H:122:GLU:HA	2.38	0.53
1:E:73:VAL:CG1	1:E:75:GLN:HE21	2.21	0.52
1:H:27:PHE:CD1	1:H:89:LEU:HD11	2.44	0.52
1:C:10:ILE:HA	1:C:116:VAL:HG22	1.92	0.52
1:E:27:PHE:CD1	1:E:89:LEU:HD11	2.43	0.52
1:E:9:ILE:O	1:E:116:VAL:HG13	2.09	0.52
1:C:90:MET:HE1	1:C:118:GLY:HA3	1.90	0.52
1:C:3:LEU:HD12	1:C:3:LEU:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:90:MET:HE3	1:F:116:VAL:HG23	1.91	0.52
1:D:46:GLU:O	1:D:48:GLY:N	2.43	0.52
1:H:89:LEU:C	1:H:89:LEU:HD12	2.34	0.52
1:G:6:THR:HB	1:G:83:ILE:HD13	1.90	0.51
1:F:41:GLN:O	1:F:41:GLN:HG3	2.10	0.51
1:G:89:LEU:HD12	1:G:89:LEU:C	2.35	0.51
1:D:19:VAL:HG12	1:D:19:VAL:O	2.11	0.51
1:E:86:ASN:C	1:E:86:ASN:HD22	2.18	0.51
1:C:27:PHE:CD1	1:C:89:LEU:HD11	2.45	0.51
1:G:9:ILE:O	1:G:116:VAL:HG13	2.11	0.51
1:G:3:LEU:O	1:G:3:LEU:HD12	2.10	0.51
1:C:58:PRO:C	1:C:59:PHE:CD1	2.88	0.51
1:F:4:GLN:CD	1:F:83:ILE:HB	2.31	0.51
1:B:9:ILE:O	1:B:116:VAL:HG13	2.11	0.50
1:C:58:PRO:O	1:C:59:PHE:C	2.53	0.50
1:C:57:ARG:NH1	1:H:58:PRO:CA	2.74	0.50
1:H:1:MET:SD	1:H:2:ALA:N	2.83	0.50
1:A:58:PRO:CG	1:E:53:GLU:O	2.60	0.50
1:B:142:ILE:O	1:B:143:ARG:O	2.30	0.50
1:D:59:PHE:H	1:D:59:PHE:HD1	1.55	0.50
1:B:57:ARG:HG2	1:B:59:PHE:CZ	2.47	0.50
1:D:9:ILE:O	1:D:116:VAL:HG13	2.12	0.49
1:A:43:SER:N	1:A:46:GLU:HG3	2.25	0.49
1:E:50:PHE:C	1:E:50:PHE:HD1	2.19	0.49
1:F:81:ASP:O	1:F:82:ALA:HB3	2.11	0.49
1:C:5:ARG:NE	1:C:78:GLU:OE1	2.46	0.49
1:C:58:PRO:C	1:C:59:PHE:O	2.56	0.49
1:B:141:ARG:NH1	1:C:15:VAL:HG13	2.27	0.49
1:A:9:ILE:O	1:A:116:VAL:HG13	2.13	0.48
1:A:135:ALA:HB3	1:G:131:TYR:HA	1.94	0.48
1:F:94:ASP:CB	1:F:111:ILE:CD1	2.90	0.48
1:F:27:PHE:CE1	1:F:89:LEU:HD11	2.48	0.48
1:B:59:PHE:C	1:B:59:PHE:CD1	2.92	0.48
1:F:10:ILE:HA	1:F:116:VAL:HG12	1.95	0.48
1:B:3:LEU:HD12	1:B:3:LEU:O	2.14	0.48
1:C:9:ILE:C	1:C:116:VAL:HG13	2.38	0.47
1:D:57:ARG:HG3	1:D:58:PRO:CD	2.44	0.47
1:D:48:GLY:CA	1:D:51:TYR:H	2.24	0.47
1:H:141:ARG:HH21	1:H:141:ARG:HG3	1.79	0.47
1:C:60:PHE:O	1:C:61:LYS:CB	2.56	0.47
1:D:27:PHE:CD1	1:D:89:LEU:HD11	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:33:ARG:N	1:F:78:GLU:O	2.38	0.47
1:C:55:LYS:N	1:C:55:LYS:HE2	2.29	0.47
1:B:142:ILE:HG22	1:B:143:ARG:N	2.30	0.47
1:A:22:GLU:O	1:A:25:THR:HG22	2.15	0.46
1:E:104:ARG:O	1:E:108:ALA:HB3	2.15	0.46
1:D:57:ARG:HG3	1:D:58:PRO:HD2	1.96	0.46
1:A:34:VAL:HG13	1:A:75:GLN:NE2	2.30	0.46
1:D:3:LEU:HD12	1:D:3:LEU:C	2.41	0.46
1:A:34:VAL:HG13	1:A:75:GLN:HE22	1.81	0.46
1:A:140:GLU:OE1	1:A:140:GLU:N	2.46	0.46
1:G:59:PHE:O	1:G:60:PHE:C	2.58	0.46
1:B:135:ALA:O	1:B:138:VAL:CG2	2.63	0.46
1:A:43:SER:OG	1:A:46:GLU:HG2	2.15	0.46
1:E:50:PHE:CE2	1:E:132:PHE:CE2	3.00	0.46
1:G:22:GLU:O	1:G:25:THR:HG22	2.16	0.46
1:A:58:PRO:HG2	1:E:53:GLU:O	2.16	0.46
1:A:104:ARG:O	1:A:108:ALA:HB3	2.16	0.46
1:D:95:PRO:HB3	1:D:108:ALA:HB3	1.98	0.46
1:G:45:ARG:CG	1:G:45:ARG:NH1	2.68	0.46
1:G:104:ARG:O	1:G:108:ALA:HB3	2.16	0.46
1:B:99:ASP:OD1	1:B:100:ALA:N	2.49	0.45
1:D:22:GLU:O	1:D:25:THR:HG22	2.16	0.45
1:E:3:LEU:O	1:E:3:LEU:HD12	2.16	0.45
1:F:80:GLU:C	1:F:81:ASP:OD1	2.58	0.45
1:H:104:ARG:O	1:H:108:ALA:HB3	2.16	0.45
1:G:57:ARG:HB3	1:G:59:PHE:CE1	2.51	0.45
1:B:27:PHE:CE1	1:B:89:LEU:HD11	2.52	0.45
1:C:53:GLU:O	1:C:54:HIS:CG	2.69	0.45
1:D:26:ARG:HG3	1:D:103:ILE:HD11	1.97	0.45
1:D:99:ASP:OD1	1:D:100:ALA:N	2.49	0.45
1:E:45:ARG:HH11	1:E:45:ARG:HD2	1.56	0.45
1:C:27:PHE:CE1	1:C:89:LEU:HD11	2.52	0.45
1:A:141:ARG:HH21	1:A:141:ARG:HG3	1.81	0.45
1:C:131:TYR:HA	1:E:135:ALA:HB3	1.99	0.45
1:G:27:PHE:CE1	1:G:89:LEU:HD11	2.52	0.45
1:H:27:PHE:CE1	1:H:89:LEU:HD11	2.51	0.45
1:A:80:GLU:O	1:A:81:ASP:OD1	2.35	0.44
1:A:58:PRO:CB	1:E:52:ALA:O	2.65	0.44
1:D:122:GLU:OE1	1:D:122:GLU:N	2.50	0.44
1:F:104:ARG:O	1:F:108:ALA:HB3	2.18	0.44
1:H:142:ILE:HD12	1:H:142:ILE:HA	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ARG:CG	1:B:143:ARG:HH11	2.30	0.44
1:C:9:ILE:O	1:C:116:VAL:CG1	2.61	0.44
1:D:104:ARG:O	1:D:108:ALA:HB3	2.16	0.44
1:E:22:GLU:O	1:E:25:THR:HG22	2.17	0.44
1:H:57:ARG:HD2	1:H:58:PRO:CD	2.47	0.44
1:A:113:GLU:OE1	1:E:122:GLU:HG2	2.16	0.44
1:B:104:ARG:O	1:B:108:ALA:HB3	2.17	0.44
1:B:139:CYS:SG	1:C:71:PRO:HB3	2.58	0.44
1:C:58:PRO:O	1:C:58:PRO:HD2	2.16	0.44
1:D:1:MET:HE3	1:D:1:MET:HB2	1.89	0.44
1:A:97:LYS:O	1:A:97:LYS:HG2	2.18	0.44
1:A:142:ILE:O	1:A:143:ARG:C	2.60	0.44
1:C:53:GLU:O	1:C:54:HIS:ND1	2.51	0.44
1:B:22:GLU:O	1:B:25:THR:HG22	2.18	0.43
1:C:104:ARG:O	1:C:108:ALA:HB3	2.18	0.43
1:E:27:PHE:CE1	1:E:89:LEU:HD11	2.53	0.43
1:F:45:ARG:HA	1:F:45:ARG:HD3	1.87	0.43
1:F:143:ARG:HG3	1:F:143:ARG:NH1	2.26	0.43
1:B:135:ALA:O	1:B:138:VAL:HG23	2.18	0.43
1:C:45:ARG:HG3	1:C:45:ARG:NH1	2.09	0.43
1:D:140:GLU:OE1	1:D:140:GLU:N	2.48	0.43
1:A:75:GLN:HE21	1:A:75:GLN:HB3	1.56	0.43
1:E:56:GLU:H	1:E:56:GLU:HG3	1.69	0.43
1:B:57:ARG:HG3	1:B:58:PRO:CD	2.42	0.43
1:E:95:PRO:HB3	1:E:108:ALA:HB3	2.00	0.43
1:E:141:ARG:HG3	1:E:141:ARG:NH2	2.30	0.43
1:A:90:MET:HE1	1:A:117:HIS:O	2.19	0.43
1:F:34:VAL:HG13	1:F:75:GLN:HE22	1.84	0.43
1:F:75:GLN:HE21	1:F:75:GLN:HB3	1.53	0.42
1:B:139:CYS:SG	1:C:71:PRO:CB	3.07	0.42
1:H:59:PHE:CD1	1:H:59:PHE:N	2.86	0.42
1:D:19:VAL:HG13	1:D:107:PHE:CE1	2.51	0.42
1:E:22:GLU:CG	1:F:25:THR:HG23	2.50	0.42
1:F:90:MET:HE3	1:F:116:VAL:CG2	2.49	0.42
1:B:3:LEU:HD12	1:B:3:LEU:C	2.44	0.42
1:C:57:ARG:CZ	1:H:58:PRO:HG3	2.47	0.42
1:F:59:PHE:CD1	1:F:59:PHE:C	2.98	0.42
1:G:52:ALA:O	1:G:55:LYS:HB2	2.19	0.42
1:B:97:LYS:O	1:B:97:LYS:HG2	2.20	0.42
1:E:30:ALA:HB1	1:E:85:LYS:HE3	2.02	0.42
1:G:3:LEU:HD12	1:G:3:LEU:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ILE:CG2	1:A:143:ARG:N	2.83	0.41
1:C:22:GLU:O	1:C:25:THR:HG22	2.19	0.41
1:B:30:ALA:HB1	1:B:85:LYS:HE2	2.02	0.41
1:E:10:ILE:HD12	1:E:23:ILE:HG21	2.03	0.41
1:G:142:ILE:HD12	1:G:142:ILE:HA	1.82	0.41
1:C:52:ALA:C	1:C:54:HIS:N	2.77	0.41
1:D:7:LEU:HD22	1:D:128:GLU:HB3	2.03	0.41
1:C:142:ILE:HD12	1:C:142:ILE:C	2.44	0.41
1:H:10:ILE:HD12	1:H:23:ILE:HG21	2.02	0.41
1:G:1:MET:HB2	1:G:1:MET:HE3	1.76	0.41
1:E:50:PHE:HE2	1:E:132:PHE:HE2	1.63	0.41
1:A:112:ASP:HB2	1:E:121:SER:HB3	2.02	0.41
1:D:10:ILE:HD12	1:D:23:ILE:HG21	2.02	0.41
1:G:86:ASN:C	1:G:86:ASN:HD22	2.29	0.41
1:D:4:GLN:OE1	1:D:83:ILE:HG22	2.20	0.40
1:G:141:ARG:HG3	1:G:141:ARG:HH21	1.86	0.40
1:C:57:ARG:HD2	1:C:57:ARG:HA	1.95	0.40
1:C:14:ALA:O	1:C:19:VAL:HG22	2.21	0.40
1:F:5:ARG:HG2	1:F:78:GLU:HB2	2.03	0.40
1:F:95:PRO:HB3	1:F:108:ALA:HB3	2.03	0.40
1:G:24:LEU:HD21	1:G:75:GLN:OE1	2.21	0.40
1:D:24:LEU:CD2	1:D:75:GLN:HE22	2.32	0.40
1:E:14:ALA:O	1:E:19:VAL:HG22	2.21	0.40
1:H:14:ALA:O	1:H:19:VAL:HG22	2.21	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:GLU:OE2	1:E:61:LYS:NZ[1_545]	1.56	0.64
1:B:53:GLU:O	1:G:58:PRO:CB[1_665]	1.66	0.54
1:A:53:GLU:O	1:F:58:PRO:CB[1_455]	1.78	0.42
1:C:60:PHE:O	1:G:120:ASP:O[1_655]	1.83	0.37
1:A:53:GLU:O	1:F:58:PRO:CA[1_455]	1.98	0.22
1:D:57:ARG:NH1	1:E:58:PRO:CA[1_545]	2.04	0.16
1:A:56:GLU:OE2	1:F:56:GLU:O[1_455]	2.08	0.12
1:B:53:GLU:O	1:G:58:PRO:CG[1_665]	2.19	0.01

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	141/143 (99%)	135 (96%)	6 (4%)	0	100	100
1	B	141/143 (99%)	137 (97%)	4 (3%)	0	100	100
1	C	141/143 (99%)	129 (92%)	7 (5%)	5 (4%)	3	23
1	D	141/143 (99%)	137 (97%)	2 (1%)	2 (1%)	9	38
1	E	141/143 (99%)	138 (98%)	3 (2%)	0	100	100
1	F	141/143 (99%)	133 (94%)	6 (4%)	2 (1%)	9	38
1	G	141/143 (99%)	136 (96%)	4 (3%)	1 (1%)	18	51
1	H	141/143 (99%)	137 (97%)	4 (3%)	0	100	100
All	All	1128/1144 (99%)	1082 (96%)	36 (3%)	10 (1%)	14	47

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	57	ARG
1	C	58	PRO
1	C	59	PHE
1	C	63	LEU
1	D	47	ALA
1	G	60	PHE
1	F	81	ASP
1	F	84	ALA
1	D	142	ILE
1	C	142	ILE

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	113/113 (100%)	104 (92%)	9 (8%)	11	36
1	B	113/113 (100%)	107 (95%)	6 (5%)	20	47
1	C	113/113 (100%)	92 (81%)	21 (19%)	1	9
1	D	113/113 (100%)	106 (94%)	7 (6%)	16	44
1	E	113/113 (100%)	101 (89%)	12 (11%)	6	28
1	F	113/113 (100%)	105 (93%)	8 (7%)	13	40
1	G	113/113 (100%)	103 (91%)	10 (9%)	9	33
1	H	113/113 (100%)	104 (92%)	9 (8%)	11	36
All	All	904/904 (100%)	822 (91%)	82 (9%)	9	33

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	25	THR
1	A	44	GLU
1	A	46	GLU
1	A	56	GLU
1	A	87	ARG
1	A	96	LYS
1	A	127	ARG
1	A	143	ARG
1	B	25	THR
1	B	56	GLU
1	B	57	ARG
1	B	138	VAL
1	B	139	CYS
1	B	143	ARG
1	C	1	MET
1	C	4	GLN
1	C	5	ARG
1	C	8	SER
1	C	18	ASN
1	C	25	THR
1	C	41	GLN
1	C	44	GLU
1	C	45	ARG

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Mol	Chain	Res	Type
1	C	55	LYS
1	C	56	GLU
1	C	57	ARG
1	C	58	PRO
1	C	59	PHE
1	C	62	ASP
1	C	111	ILE
1	C	117	HIS
1	C	120	ASP
1	C	137	GLU
1	C	142	ILE
1	C	143	ARG
1	D	1	MET
1	D	25	THR
1	D	41	GLN
1	D	56	GLU
1	D	57	ARG
1	D	142	ILE
1	D	143	ARG
1	E	5	ARG
1	E	25	THR
1	E	33	ARG
1	E	44	GLU
1	E	50	PHE
1	E	56	GLU
1	E	93	THR
1	E	96	LYS
1	E	99	ASP
1	E	124	SER
1	E	141	ARG
1	E	143	ARG
1	F	41	GLN
1	F	56	GLU
1	F	80	GLU
1	F	85	LYS
1	F	116	VAL
1	F	120	ASP
1	F	137	GLU
1	F	140	GLU
1	G	1	MET
1	G	25	THR
1	G	34	VAL

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Mol	Chain	Res	Type
1	G	41	GLN
1	G	46	GLU
1	G	57	ARG
1	G	59	PHE
1	G	86	ASN
1	G	96	LYS
1	G	143	ARG
1	H	1	MET
1	H	4	GLN
1	H	41	GLN
1	H	55	LYS
1	H	59	PHE
1	H	64	VAL
1	H	87	ARG
1	H	124	SER
1	H	143	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	75	GLN
1	A	117	HIS
1	B	41	GLN
1	B	75	GLN
1	B	86	ASN
1	B	117	HIS
1	C	18	ASN
1	C	86	ASN
1	C	117	HIS
1	D	75	GLN
1	D	86	ASN
1	D	117	HIS
1	E	18	ASN
1	E	41	GLN
1	E	54	HIS
1	E	75	GLN
1	E	117	HIS
1	F	75	GLN
1	F	117	HIS
1	G	117	HIS
1	H	117	HIS

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](#)

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	A	143/143 (100%)	0.30	2 (1%) 73 45	63, 97, 160, 201	0
1	B	143/143 (100%)	0.31	2 (1%) 73 45	69, 106, 164, 215	0
1	C	143/143 (100%)	0.35	2 (1%) 73 45	67, 106, 151, 225	0
1	D	143/143 (100%)	0.43	5 (3%) 47 26	69, 118, 155, 197	0
1	E	143/143 (100%)	0.35	3 (2%) 63 36	62, 105, 164, 202	0
1	F	143/143 (100%)	0.27	2 (1%) 73 45	65, 118, 182, 258	0
1	G	143/143 (100%)	0.38	4 (2%) 55 30	66, 110, 161, 200	0
1	H	143/143 (100%)	0.32	1 (0%) 84 61	75, 110, 153, 183	0
All	All	1144/1144 (100%)	0.34	21 (1%) 67 40	62, 108, 168, 258	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	68	THR	6.1
1	G	93	THR	3.7
1	A	108	ALA	3.4
1	E	68	THR	3.0
1	B	122	GLU	2.9
1	D	116	VAL	2.5
1	F	57	ARG	2.5
1	C	116	VAL	2.5
1	G	115	ALA	2.4
1	D	65	SER	2.3
1	E	58	PRO	2.3
1	D	56	GLU	2.3
1	D	115	ALA	2.3
1	B	1	MET	2.3
1	E	124	SER	2.2
1	C	115	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	7	LEU	2.1
1	F	75	GLN	2.1
1	G	113	GLU	2.0
1	A	98	ALA	2.0
1	H	34	VAL	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.