Full wwPDB X-ray Structure Validation Report ⓘ

Dec 21, 2024 – 04:30 pm GMT

PDB ID	:	8RJH
Title	:	HLA A*2402-NF9_6F pMHC complex
Authors	:	Wall, A.; Sewell, A.K.; Motozono, C.; Rizkallah, P.J.; Fuller, A.
Deposited on	:	2023-12-21
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

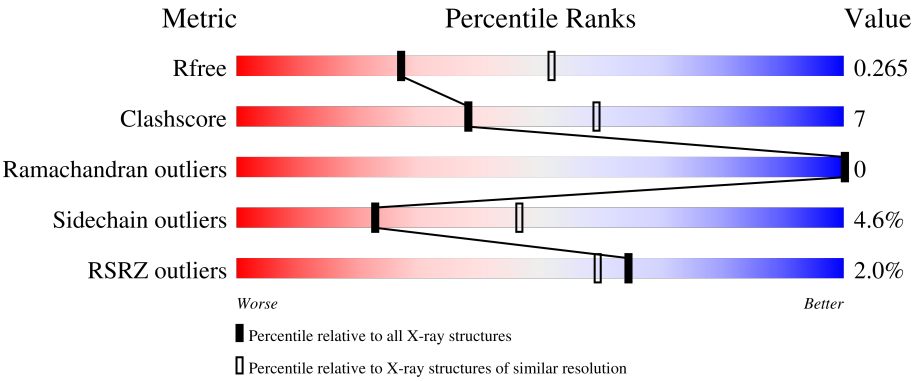
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	276	4% 82% 18%
1	D	276	% 83% 17%
1	G	276	3% 81% 18%
1	J	276	3% 85% 14%
1	M	276	2% 85% 15%

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Mol	Chain	Length	Quality of chain
1	P	276	2% 84% 16%
2	B	100	2% 87% 12%
2	E	100	83% 14%
2	H	100	85% 12%
2	K	100	79% 18%
2	N	100	85% 12%
2	Q	100	92% 6%
3	C	9	56% 44%
3	F	9	11% 67% 22% 11%
3	I	9	11% 56% 33% 11%
3	L	9	33% 44% 22%
3	O	9	67% 22% 11%
3	R	9	89% 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 19159 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2238	1392	405	431	10			
1	D	276	Total	C	N	O	S	0	0	0
			2238	1392	405	431	10			
1	G	276	Total	C	N	O	S	0	0	0
			2238	1392	405	431	10			
1	J	276	Total	C	N	O	S	0	0	0
			2238	1392	405	431	10			
1	M	276	Total	C	N	O	S	0	0	0
			2238	1392	405	431	10			
1	P	276	Total	C	N	O	S	0	0	0
			2238	1392	405	431	10			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	E	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	H	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	K	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	N	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	Q	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769

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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	MET	-	initiating methionine	UNP P61769
H	0	MET	-	initiating methionine	UNP P61769
K	0	MET	-	initiating methionine	UNP P61769
N	0	MET	-	initiating methionine	UNP P61769
Q	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called ASN-TYR-ASN-TYR-LEU-PHE-ARG-LEU-PHE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			90	62	14	14			
3	F	9	Total	C	N	O	0	0	0
			90	62	14	14			
3	I	9	Total	C	N	O	0	0	0
			90	62	14	14			
3	L	9	Total	C	N	O	0	0	0
			90	62	14	14			
3	O	9	Total	C	N	O	0	0	0
			90	62	14	14			
3	R	9	Total	C	N	O	0	0	0
			90	62	14	14			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	O	0	0
			15	15		
4	B	11	Total	O	0	0
			11	11		
4	D	12	Total	O	0	0
			12	12		
4	E	17	Total	O	0	0
			17	17		
4	F	1	Total	O	0	0
			1	1		
4	G	18	Total	O	0	0
			18	18		
4	H	6	Total	O	0	0
			6	6		
4	J	7	Total	O	0	0
			7	7		
4	K	15	Total	O	0	0
			15	15		

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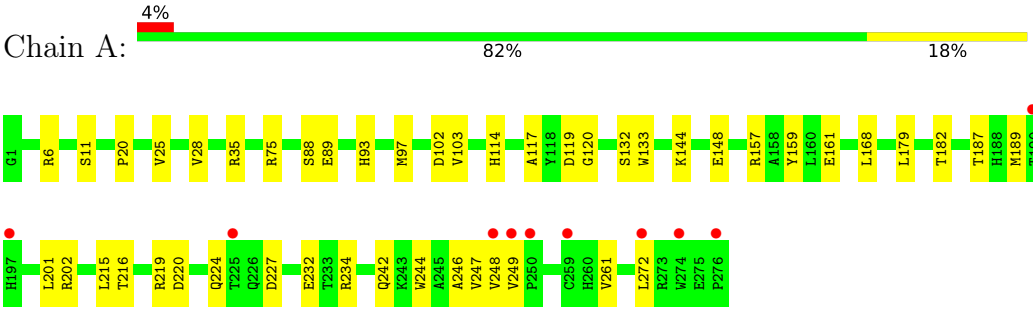
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	18	Total O 18 18	0	0
4	N	16	Total O 16 16	0	0
4	P	14	Total O 14 14	0	0
4	Q	18	Total O 18 18	0	0
4	R	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

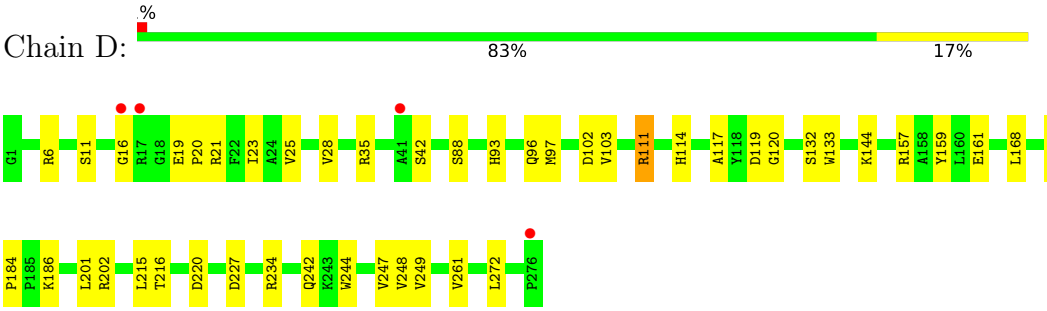
• Molecule 1: MHC class I antigen

Chain A:



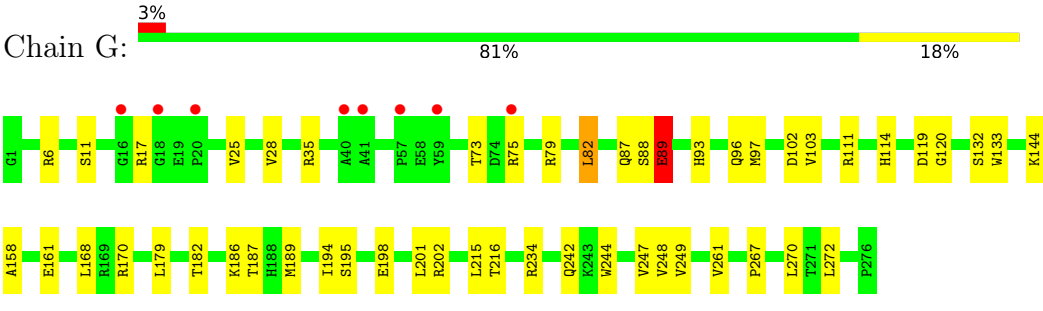
• Molecule 1: MHC class I antigen

Chain D:



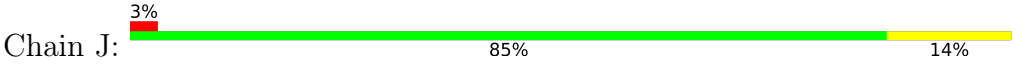
• Molecule 1: MHC class I antigen

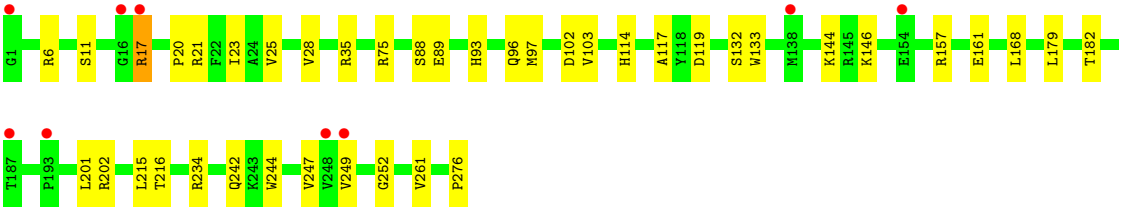
Chain G:



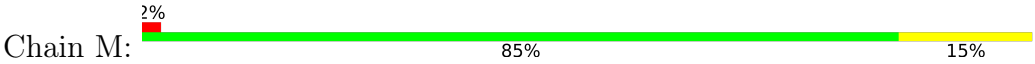
• Molecule 1: MHC class I antigen

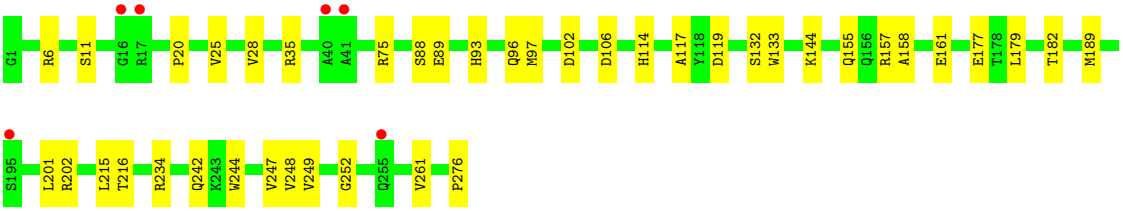
Chain J:



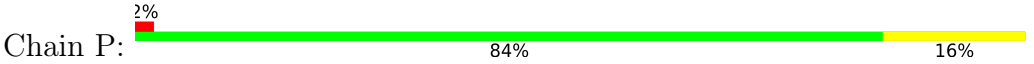


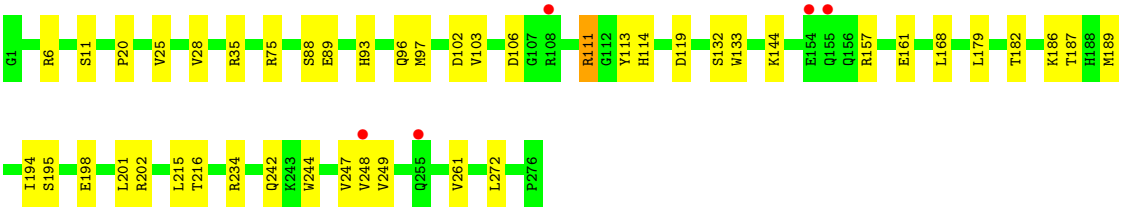
• Molecule 1: MHC class I antigen



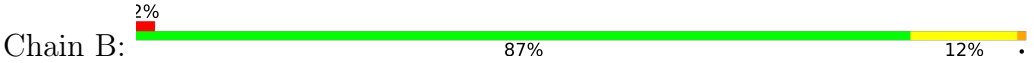


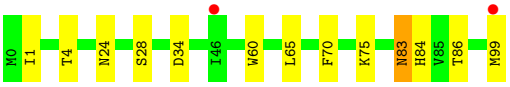
• Molecule 1: MHC class I antigen



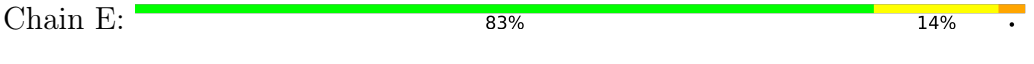


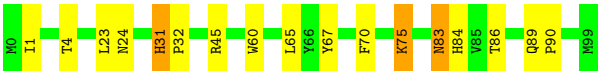
• Molecule 2: Beta-2-microglobulin



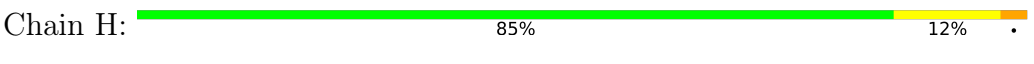


• Molecule 2: Beta-2-microglobulin



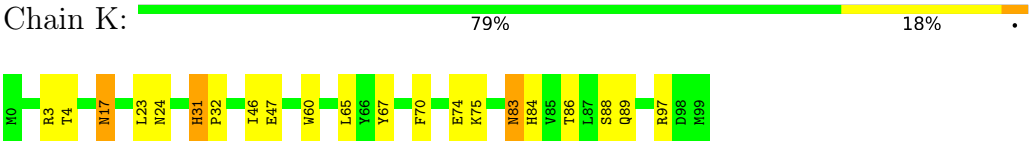


• Molecule 2: Beta-2-microglobulin



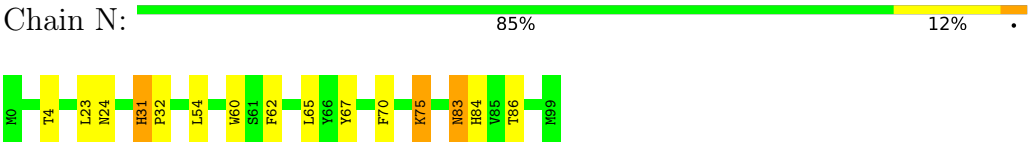
• Molecule 2: Beta-2-microglobulin

Chain K:



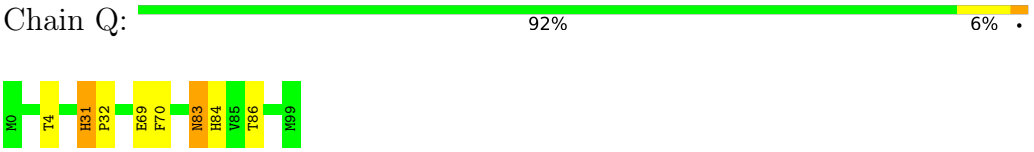
• Molecule 2: Beta-2-microglobulin

Chain N:



• Molecule 2: Beta-2-microglobulin

Chain Q:

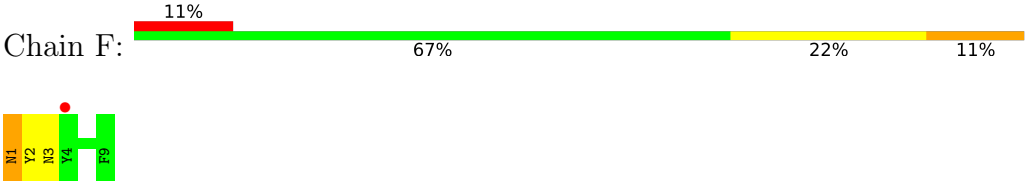


• Molecule 3: ASN-TYR-ASN-TYR-LEU-PHE-ARG-LEU-PHE

Chain C:

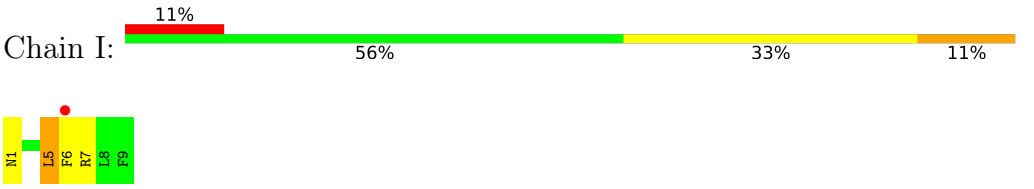
• Molecule 3: ASN-TYR-ASN-TYR-LEU-PHE-ARG-LEU-PHE

Chain F:



• Molecule 3: ASN-TYR-ASN-TYR-LEU-PHE-ARG-LEU-PHE

Chain I:

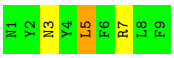


• Molecule 3: ASN-TYR-ASN-TYR-LEU-PHE-ARG-LEU-PHE

Chain L:

• Molecule 3: ASN-TYR-ASN-TYR-LEU-PHE-ARG-LEU-PHE

Chain O:



• Molecule 3: ASN-TYR-ASN-TYR-LEU-PHE-ARG-LEU-PHE

Chain R:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	344.80Å 84.34Å 91.45Å 90.00° 102.14° 90.00°	Depositor
Resolution (Å)	87.00 – 2.60 87.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (87.00-2.60) 99.9 (87.00-2.60)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.224 , 0.264 0.225 , 0.265	Depositor DCC
R_{free} test set	3967 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	48.3	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19159	wwPDB-VP
Average B, all atoms (Å^2)	67.0	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 31.85 % 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 1.0342e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.73	1/2299 (0.0%)	0.79	0/3116
1	D	0.71	0/2299	0.77	1/3116 (0.0%)
1	G	0.72	1/2299 (0.0%)	0.78	0/3116
1	J	0.71	0/2299	0.77	0/3116
1	M	0.70	0/2299	0.78	0/3116
1	P	0.71	0/2299	0.77	0/3116
2	B	0.76	0/860	0.77	0/1162
2	E	0.70	0/860	0.77	0/1162
2	H	0.73	0/860	0.78	0/1162
2	K	0.70	0/860	0.78	0/1162
2	N	0.73	0/860	0.78	0/1162
2	Q	0.72	0/860	0.75	0/1162
3	C	0.66	0/93	1.12	0/123
3	F	0.61	0/93	0.89	0/123
3	I	0.86	0/93	1.01	0/123
3	L	0.61	0/93	0.98	0/123
3	O	0.68	0/93	0.80	0/123
3	R	0.74	0/93	0.96	0/123
All	All	0.71	2/19512 (0.0%)	0.78	1/26406 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	89	GLU	CD-OE1	5.54	1.31	1.25
1	A	148	GLU	CD-OE1	5.37	1.31	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	111	ARG	CG-CD-NE	5.21	122.75	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2238	0	2095	37	0
1	D	2238	0	2095	28	1
1	G	2238	0	2095	41	0
1	J	2238	0	2095	27	0
1	M	2238	0	2095	34	0
1	P	2238	0	2095	24	0
2	B	837	0	803	12	0
2	E	837	0	803	20	0
2	H	837	0	803	15	0
2	K	837	0	803	19	0
2	N	837	0	803	13	0
2	Q	837	0	803	8	0
3	C	90	0	85	7	0
3	F	90	0	85	2	0
3	I	90	0	85	8	0
3	L	90	0	85	4	0
3	O	90	0	85	5	0
3	R	90	0	85	0	0
4	A	15	0	0	0	0
4	B	11	0	0	1	0
4	D	12	0	0	0	0
4	E	17	0	0	2	0
4	F	1	0	0	0	0
4	G	18	0	0	0	0
4	H	6	0	0	0	0
4	J	7	0	0	0	0
4	K	15	0	0	2	0
4	M	18	0	0	0	0
4	N	16	0	0	0	0
4	P	14	0	0	0	0
4	Q	18	0	0	1	0
4	R	1	0	0	0	0
All	All	19159	0	17898	251	1

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 7.

All (251) 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:G:267:PRO:HG3	1:M:276:PRO:HG2	1.36	1.08
1:M:155:GLN:HE22	3:O:7:ARG:HH11	1.16	0.90
1:G:267:PRO:CG	1:M:276:PRO:HG2	2.06	0.86
2:E:75:LYS:HE2	4:E:117:HOH:O	1.75	0.84
1:G:267:PRO:HG3	1:M:276:PRO:CG	2.07	0.83
2:H:83:ASN:HD22	2:H:84:HIS:H	1.30	0.80
2:E:89:GLN:HG2	2:E:90:PRO:HD2	1.64	0.79
1:M:6:ARG:NH2	1:M:102:ASP:OD1	2.15	0.78
1:A:6:ARG:NH2	1:A:102:ASP:OD1	2.16	0.78
1:P:6:ARG:NH2	1:P:102:ASP:OD1	2.16	0.78
2:E:83:ASN:HD22	2:E:84:HIS:H	1.32	0.78
1:G:267:PRO:CG	1:M:276:PRO:CG	2.62	0.77
2:Q:83:ASN:HD22	2:Q:84:HIS:H	1.33	0.77
1:G:6:ARG:NH2	1:G:102:ASP:OD1	2.17	0.77
2:N:83:ASN:HD22	2:N:84:HIS:H	1.32	0.76
1:D:6:ARG:NH2	1:D:102:ASP:OD1	2.19	0.76
1:J:6:ARG:NH2	1:J:102:ASP:OD1	2.19	0.76
2:B:83:ASN:HD22	2:B:84:HIS:H	1.32	0.76
2:K:83:ASN:HD22	2:K:84:HIS:H	1.36	0.72
1:P:157:ARG:NH1	1:P:161:GLU:OE2	2.23	0.72
1:A:159:TYR:CD1	3:C:3:ASN:HB3	2.26	0.70
1:M:157:ARG:NH1	1:M:161:GLU:OE2	2.25	0.70
1:A:157:ARG:NH1	1:A:161:GLU:OE2	2.25	0.69
1:D:157:ARG:NH1	1:D:161:GLU:OE2	2.25	0.69
1:J:157:ARG:NH1	1:J:161:GLU:OE2	2.25	0.69
1:G:157:ARG:NH1	1:G:161:GLU:OE2	2.26	0.69
3:L:3:ASN:HD22	3:L:4:TYR:H	1.41	0.68
1:G:120:GLY:O	2:H:1:ILE:HD12	1.93	0.68
1:D:120:GLY:O	2:E:1:ILE:HD12	1.94	0.66
1:A:187:THR:HB	1:A:272:LEU:HD11	1.76	0.65
1:A:159:TYR:CE1	3:C:3:ASN:HB3	2.31	0.64
2:E:75:LYS:HE3	2:E:75:LYS:O	1.97	0.64
1:J:96:GLN:OE1	2:K:31:HIS:HE1	1.80	0.63
2:Q:69:GLU:HB2	4:Q:109:HOH:O	1.97	0.63
3:O:5:LEU:HG	3:O:5:LEU:O	1.98	0.63
1:G:170:ARG:HH22	3:I:1:ASN:HD21	1.49	0.61
2:N:75:LYS:O	2:N:75:LYS:HE3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:73:THR:HG21	3:I:6:PHE:HB2	1.82	0.61
1:M:234:ARG:HE	1:M:242:GLN:HE21	1.50	0.60
2:B:83:ASN:HD22	2:B:84:HIS:N	1.99	0.60
3:I:6:PHE:O	3:I:7:ARG:HD2	2.02	0.60
1:M:93:HIS:HD2	1:M:119:ASP:OD2	1.85	0.59
1:G:93:HIS:HD2	1:G:119:ASP:OD2	1.85	0.59
1:G:155:GLN:HB3	3:I:5:LEU:CD2	2.33	0.59
1:A:159:TYR:CG	3:C:3:ASN:HB3	2.38	0.59
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.85	0.59
2:K:3:ARG:CD	4:K:107:HOH:O	2.51	0.59
1:J:93:HIS:HD2	1:J:119:ASP:OD2	1.85	0.58
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.39	0.58
2:H:4:THR:HG22	2:H:86:THR:OG1	2.03	0.58
2:B:4:THR:HG22	2:B:86:THR:OG1	2.03	0.58
1:P:93:HIS:HD2	1:P:119:ASP:OD2	1.86	0.57
1:D:93:HIS:HD2	1:D:119:ASP:OD2	1.86	0.57
2:Q:83:ASN:HD22	2:Q:84:HIS:N	2.01	0.57
1:G:82:LEU:CD2	1:G:87:GLN:HB2	2.35	0.57
1:G:234:ARG:HE	1:G:242:GLN:HE21	1.52	0.57
1:J:202:ARG:HD2	1:J:244:TRP:CD2	2.40	0.57
1:P:234:ARG:HE	1:P:242:GLN:HE21	1.53	0.57
2:K:4:THR:HG22	2:K:86:THR:OG1	2.05	0.57
1:D:184:PRO:HG2	1:J:276:PRO:HG2	1.87	0.57
1:M:155:GLN:NE2	3:O:7:ARG:HH11	1.95	0.57
2:H:75:LYS:HE3	2:H:75:LYS:O	2.05	0.56
2:N:4:THR:HG22	2:N:86:THR:OG1	2.04	0.56
2:E:4:THR:HG22	2:E:86:THR:OG1	2.06	0.56
2:K:83:ASN:HD22	2:K:84:HIS:N	2.03	0.56
2:E:89:GLN:HG2	2:E:90:PRO:CD	2.35	0.56
2:E:83:ASN:HD22	2:E:84:HIS:N	2.03	0.56
1:G:82:LEU:HD22	1:G:87:GLN:HB2	1.87	0.55
1:D:234:ARG:HE	1:D:242:GLN:HE21	1.54	0.55
1:G:96:GLN:OE1	2:H:31:HIS:HE1	1.89	0.55
1:P:202:ARG:HD2	1:P:244:TRP:CD2	2.41	0.55
2:Q:4:THR:HG22	2:Q:86:THR:OG1	2.05	0.55
1:A:220:ASP:OD2	1:M:106:ASP:HB3	2.06	0.55
1:G:187:THR:HB	1:G:272:LEU:HD11	1.88	0.55
1:P:96:GLN:OE1	2:Q:31:HIS:HE1	1.90	0.54
1:M:155:GLN:HE22	3:O:7:ARG:NH1	1.95	0.54
1:A:232:GLU:OE1	2:B:28:SER:OG	2.24	0.54
1:D:96:GLN:OE1	2:E:31:HIS:HE1	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:ARG:HD2	1:D:244:TRP:CD2	2.43	0.54
2:K:3:ARG:HD2	4:K:107:HOH:O	2.07	0.54
1:M:20:PRO:HG2	1:M:75:ARG:HD3	1.90	0.54
1:D:220:ASP:CG	1:P:106:ASP:HB3	2.28	0.54
2:K:46:ILE:HG22	2:K:47:GLU:O	2.09	0.53
1:J:96:GLN:OE1	2:K:31:HIS:CE1	2.60	0.53
2:N:83:ASN:HD22	2:N:84:HIS:N	2.02	0.53
1:A:234:ARG:HE	1:A:242:GLN:HE21	1.57	0.52
1:P:111:ARG:NH2	1:P:113:TYR:OH	2.42	0.52
1:G:202:ARG:HD2	1:G:244:TRP:CD2	2.44	0.52
1:A:159:TYR:CD1	3:C:3:ASN:CB	2.93	0.52
3:L:3:ASN:HD22	3:L:4:TYR:N	2.07	0.52
1:M:97:MET:CE	1:M:114:HIS:CE1	2.93	0.52
1:A:194:ILE:HG13	1:A:195:SER:N	2.25	0.52
1:G:194:ILE:HG13	1:G:195:SER:N	2.24	0.52
2:H:83:ASN:HD22	2:H:84:HIS:N	2.02	0.51
1:J:146:LYS:HE2	3:L:9:PHE:O	2.09	0.51
1:A:97:MET:CE	1:A:114:HIS:CE1	2.94	0.51
1:M:201:LEU:HD12	1:M:249:VAL:HG21	1.93	0.51
1:P:97:MET:CE	1:P:114:HIS:CE1	2.94	0.51
1:M:202:ARG:HD2	1:M:244:TRP:CD2	2.45	0.51
1:A:220:ASP:HB3	1:M:106:ASP:CB	2.41	0.51
1:G:79:ARG:HH12	1:G:89:GLU:HG2	1.75	0.51
1:P:215:LEU:CD2	1:P:261:VAL:HG22	2.41	0.51
1:A:215:LEU:CD2	1:A:261:VAL:HG22	2.41	0.50
2:B:4:THR:HG23	2:B:86:THR:HB	1.93	0.50
2:E:4:THR:HG23	2:E:86:THR:HB	1.92	0.50
1:J:201:LEU:HD12	1:J:249:VAL:HG21	1.92	0.50
1:M:96:GLN:OE1	2:N:31:HIS:HE1	1.94	0.50
3:L:5:LEU:HD23	3:L:7:ARG:HD3	1.93	0.50
1:G:155:GLN:HB3	3:I:5:LEU:HD22	1.93	0.50
1:P:20:PRO:HG2	1:P:75:ARG:HD3	1.94	0.50
1:G:97:MET:CE	1:G:114:HIS:CE1	2.94	0.50
2:Q:4:THR:HG23	2:Q:86:THR:HB	1.94	0.50
2:H:75:LYS:O	2:H:75:LYS:CE	2.60	0.49
1:A:97:MET:SD	3:C:6:PHE:HE1	2.35	0.49
1:J:97:MET:CE	1:J:114:HIS:CE1	2.94	0.49
1:M:215:LEU:CD2	1:M:261:VAL:HG22	2.42	0.49
1:A:202:ARG:HH21	2:B:99:MET:HG2	1.77	0.49
2:E:45:ARG:N	4:E:101:HOH:O	2.42	0.49
1:G:201:LEU:HD12	1:G:249:VAL:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:PRO:HG2	1:A:75:ARG:HD3	1.94	0.49
1:A:159:TYR:CZ	3:C:3:ASN:HB3	2.48	0.49
2:K:4:THR:HG23	2:K:86:THR:HB	1.93	0.49
1:G:215:LEU:CD2	1:G:261:VAL:HG22	2.42	0.49
1:D:215:LEU:CD2	1:D:261:VAL:HG22	2.43	0.49
2:H:4:THR:HG23	2:H:86:THR:HB	1.94	0.49
1:P:201:LEU:HD12	1:P:249:VAL:HG21	1.94	0.48
1:D:97:MET:CE	1:D:114:HIS:CE1	2.96	0.48
1:G:155:GLN:HB3	3:I:5:LEU:HD21	1.94	0.48
1:J:20:PRO:HG2	1:J:75:ARG:HD3	1.95	0.48
2:B:4:THR:CG2	2:B:86:THR:OG1	2.62	0.48
1:D:201:LEU:HD12	1:D:249:VAL:HG21	1.95	0.48
2:N:4:THR:HG23	2:N:86:THR:HB	1.95	0.48
1:D:184:PRO:HG3	1:J:276:PRO:HB2	1.95	0.47
2:H:4:THR:CG2	2:H:86:THR:OG1	2.62	0.47
1:G:248:VAL:HG23	1:G:248:VAL:O	2.14	0.47
1:D:248:VAL:HG23	1:D:248:VAL:O	2.14	0.47
2:N:75:LYS:O	2:N:75:LYS:CE	2.62	0.47
2:E:4:THR:CG2	2:E:86:THR:OG1	2.63	0.46
2:N:4:THR:CG2	2:N:86:THR:OG1	2.64	0.46
2:Q:31:HIS:CD2	2:Q:32:PRO:HA	2.50	0.46
1:P:133:TRP:HB2	1:P:144:LYS:HG3	1.97	0.46
2:Q:4:THR:CG2	2:Q:86:THR:OG1	2.63	0.46
1:J:215:LEU:CD2	1:J:261:VAL:HG22	2.45	0.46
2:K:4:THR:CG2	2:K:86:THR:OG1	2.63	0.46
1:A:201:LEU:HD12	1:A:249:VAL:HG21	1.97	0.46
1:G:79:ARG:HH12	1:G:89:GLU:CG	2.28	0.46
1:M:177:GLU:OE1	1:M:177:GLU:HA	2.15	0.46
1:P:194:ILE:HG13	1:P:195:SER:N	2.30	0.46
1:G:73:THR:CG2	3:I:6:PHE:HB2	2.46	0.46
1:J:133:TRP:HB2	1:J:144:LYS:HG3	1.96	0.45
1:A:20:PRO:HD2	1:A:75:ARG:HD3	1.98	0.45
1:A:248:VAL:O	1:A:248:VAL:HG23	2.17	0.45
1:A:189:MET:CE	1:A:201:LEU:HD22	2.46	0.45
1:D:182:THR:HG23	1:D:182:THR:O	2.16	0.45
1:D:97:MET:HE2	1:D:114:HIS:CE1	2.52	0.45
1:D:184:PRO:CG	1:J:276:PRO:HB2	2.47	0.45
2:E:75:LYS:O	2:E:75:LYS:CE	2.64	0.45
3:F:1:ASN:HD22	3:F:1:ASN:HA	1.64	0.45
1:M:117:ALA:HB2	2:N:60:TRP:CE2	2.52	0.45
1:A:97:MET:HE2	1:A:114:HIS:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:97:MET:HE2	1:J:114:HIS:CE1	2.52	0.45
1:A:182:THR:HG23	1:A:182:THR:O	2.17	0.45
1:G:120:GLY:C	2:H:1:ILE:HD12	2.37	0.45
1:A:232:GLU:CD	2:B:28:SER:OG	2.55	0.44
1:D:133:TRP:O	1:D:144:LYS:HE3	2.18	0.44
2:H:24:ASN:HB3	2:H:65:LEU:HD11	1.98	0.44
1:J:182:THR:HG23	1:J:182:THR:O	2.17	0.44
1:P:182:THR:HG23	1:P:182:THR:O	2.16	0.44
1:D:272:LEU:HD22	1:J:252:GLY:O	2.17	0.44
2:N:31:HIS:CD2	2:N:32:PRO:HA	2.52	0.44
1:P:97:MET:HE2	1:P:114:HIS:CE1	2.53	0.44
1:P:248:VAL:HG23	1:P:248:VAL:O	2.17	0.44
1:A:133:TRP:HB2	1:A:144:LYS:HG3	1.99	0.44
1:J:133:TRP:O	1:J:144:LYS:HE3	2.18	0.44
1:J:21:ARG:HE	1:J:23:ILE:HD11	1.82	0.44
1:M:97:MET:HE2	1:M:114:HIS:CE1	2.53	0.44
2:B:75:LYS:NZ	4:B:104:HOH:O	2.51	0.44
1:M:133:TRP:O	1:M:144:LYS:HE3	2.17	0.44
1:M:182:THR:HG23	1:M:182:THR:O	2.17	0.44
1:G:189:MET:CE	1:G:201:LEU:HD22	2.47	0.44
1:M:248:VAL:O	1:M:248:VAL:HG23	2.17	0.44
1:P:194:ILE:HD11	1:P:198:GLU:HB2	2.00	0.44
1:G:133:TRP:O	1:G:144:LYS:HE3	2.18	0.43
1:G:267:PRO:CG	1:M:276:PRO:HG3	2.47	0.43
2:K:88:SER:C	2:K:89:GLN:HG3	2.38	0.43
2:B:24:ASN:HB3	2:B:65:LEU:HD11	2.00	0.43
1:D:272:LEU:CD2	1:J:252:GLY:O	2.66	0.43
1:D:103:VAL:HG13	1:D:168:LEU:HD23	2.00	0.43
1:G:97:MET:HE2	1:G:114:HIS:CE1	2.53	0.43
2:E:31:HIS:CD2	2:E:32:PRO:HA	2.53	0.43
1:J:103:VAL:HG13	1:J:168:LEU:HD23	2.00	0.43
1:M:20:PRO:HG2	1:M:75:ARG:CD	2.48	0.43
1:G:133:TRP:HB2	1:G:144:LYS:HG3	2.00	0.43
1:J:117:ALA:HB2	2:K:60:TRP:CE2	2.53	0.43
1:D:133:TRP:HB2	1:D:144:LYS:HG3	2.00	0.43
1:P:133:TRP:O	1:P:144:LYS:HE3	2.18	0.43
1:D:159:TYR:CE1	3:F:3:ASN:HA	2.53	0.43
2:H:31:HIS:CD2	2:H:32:PRO:HA	2.54	0.43
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.53	0.43
1:G:182:THR:HG23	1:G:182:THR:O	2.19	0.43
1:P:20:PRO:HD2	1:P:75:ARG:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:TYR:CD2	3:C:3:ASN:HB3	2.54	0.42
1:D:96:GLN:OE1	2:E:31:HIS:CE1	2.71	0.42
2:K:31:HIS:CD2	2:K:32:PRO:HA	2.54	0.42
1:P:187:THR:HB	1:P:272:LEU:HD11	2.00	0.42
2:H:23:LEU:O	2:H:67:TYR:HA	2.20	0.42
2:K:74:GLU:O	2:K:75:LYS:HB2	2.18	0.42
1:A:28:VAL:HG11	1:A:179:LEU:HD13	2.01	0.42
1:G:194:ILE:HD11	1:G:198:GLU:HB2	2.01	0.42
1:G:96:GLN:OE1	2:H:31:HIS:CE1	2.70	0.42
2:K:17:ASN:N	2:K:17:ASN:OD1	2.52	0.42
1:A:133:TRP:O	1:A:144:LYS:HE3	2.19	0.42
1:D:28:VAL:HG11	1:D:179:LEU:HD13	2.01	0.42
1:G:270:LEU:HA	1:M:252:GLY:O	2.19	0.42
1:A:103:VAL:HG13	1:A:168:LEU:HD23	2.01	0.42
2:K:24:ASN:HB3	2:K:65:LEU:HD11	2.01	0.42
2:N:23:LEU:O	2:N:67:TYR:HA	2.20	0.42
1:M:133:TRP:HB2	1:M:144:LYS:HG3	2.01	0.42
1:P:28:VAL:HG11	1:P:179:LEU:HD13	2.02	0.41
1:G:28:VAL:HG11	1:G:179:LEU:HD13	2.02	0.41
2:K:23:LEU:O	2:K:67:TYR:HA	2.20	0.41
1:J:28:VAL:HG11	1:J:179:LEU:HD13	2.02	0.41
1:J:234:ARG:HE	1:J:242:GLN:HE21	1.67	0.41
2:E:4:THR:HG23	2:E:86:THR:CB	2.50	0.41
2:E:23:LEU:O	2:E:67:TYR:HA	2.20	0.41
1:G:155:GLN:O	1:G:158:ALA:HB3	2.21	0.41
1:J:17:ARG:HE	1:J:17:ARG:HB2	1.78	0.41
2:K:17:ASN:OD1	2:K:97:ARG:NH1	2.44	0.41
1:A:20:PRO:HG2	1:A:75:ARG:CD	2.50	0.41
1:A:201:LEU:O	1:A:246:ALA:HA	2.21	0.41
2:H:41:LYS:HD3	2:H:78:TYR:CE2	2.55	0.41
1:M:155:GLN:O	1:M:158:ALA:HB3	2.21	0.41
2:N:24:ASN:HB3	2:N:65:LEU:HD11	2.01	0.41
1:P:189:MET:CE	1:P:201:LEU:HD22	2.51	0.41
1:D:19:GLU:HB2	1:D:20:PRO:HD2	2.03	0.41
2:K:4:THR:HG23	2:K:86:THR:CB	2.51	0.41
1:G:103:VAL:HG13	1:G:168:LEU:HD23	2.03	0.41
1:M:189:MET:CE	1:M:201:LEU:HD22	2.51	0.41
2:N:54:LEU:HD11	2:N:62:PHE:CD1	2.56	0.41
1:P:103:VAL:HG13	1:P:168:LEU:HD23	2.02	0.41
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.57	0.40
1:G:73:THR:OG1	3:I:6:PHE:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:21:ARG:NE	1:J:23:ILE:HD11	2.36	0.40
1:M:20:PRO:HD2	1:M:75:ARG:HD3	2.03	0.40
1:A:120:GLY:O	2:B:1:ILE:HD12	2.21	0.40
1:D:21:ARG:HE	1:D:23:ILE:HD11	1.86	0.40
1:A:219:ARG:HB2	1:A:224:GLN:HG3	2.03	0.40
2:E:24:ASN:HB3	2:E:65:LEU:HD11	2.02	0.40
2:E:75:LYS:HE3	2:E:75:LYS:HA	2.03	0.40
1:M:28:VAL:HG11	1:M:179:LEU:HD13	2.03	0.40
1:M:155:GLN:HB3	3:O:5:LEU:HD11	2.03	0.40

All (1) 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:16:GLY:O	1:D:42:SER:O[2_555]	1.99	0.21

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	274/276 (99%)	265 (97%)	9 (3%)	0	100	100
1	D	274/276 (99%)	268 (98%)	6 (2%)	0	100	100
1	G	274/276 (99%)	267 (97%)	7 (3%)	0	100	100
1	J	274/276 (99%)	268 (98%)	6 (2%)	0	100	100
1	M	274/276 (99%)	267 (97%)	7 (3%)	0	100	100
1	P	274/276 (99%)	268 (98%)	6 (2%)	0	100	100
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	E	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	H	98/100 (98%)	96 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	N	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	Q	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
3	I	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	L	7/9 (78%)	7 (100%)	0	0	100	100
3	O	7/9 (78%)	7 (100%)	0	0	100	100
3	R	7/9 (78%)	7 (100%)	0	0	100	100
All	All	2274/2310 (98%)	2220 (98%)	54 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/232 (100%)	223 (96%)	9 (4%)	27	53
1	D	232/232 (100%)	222 (96%)	10 (4%)	25	49
1	G	232/232 (100%)	219 (94%)	13 (6%)	17	38
1	J	232/232 (100%)	223 (96%)	9 (4%)	27	53
1	M	232/232 (100%)	224 (97%)	8 (3%)	32	58
1	P	232/232 (100%)	222 (96%)	10 (4%)	25	49
2	B	95/95 (100%)	92 (97%)	3 (3%)	34	60
2	E	95/95 (100%)	91 (96%)	4 (4%)	25	50
2	H	95/95 (100%)	91 (96%)	4 (4%)	25	50
2	K	95/95 (100%)	91 (96%)	4 (4%)	25	50
2	N	95/95 (100%)	91 (96%)	4 (4%)	25	50
2	Q	95/95 (100%)	92 (97%)	3 (3%)	34	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	9/9 (100%)	7 (78%)	2 (22%)	1 1
3	F	9/9 (100%)	7 (78%)	2 (22%)	1 1
3	I	9/9 (100%)	8 (89%)	1 (11%)	5 10
3	L	9/9 (100%)	6 (67%)	3 (33%)	0 0
3	O	9/9 (100%)	7 (78%)	2 (22%)	1 1
3	R	9/9 (100%)	8 (89%)	1 (11%)	5 10
All	All	2016/2016 (100%)	1924 (95%)	92 (5%)	23 46

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	25	VAL
1	A	35	ARG
1	A	88	SER
1	A	89	GLU
1	A	132	SER
1	A	216	THR
1	A	227	ASP
1	A	247	VAL
2	B	34	ASP
2	B	70	PHE
2	B	83	ASN
3	C	4	TYR
3	C	5	LEU
1	D	11	SER
1	D	25	VAL
1	D	35	ARG
1	D	88	SER
1	D	111	ARG
1	D	132	SER
1	D	186	LYS
1	D	216	THR
1	D	227	ASP
1	D	247	VAL
2	E	31	HIS
2	E	70	PHE
2	E	75	LYS
2	E	83	ASN
3	F	1	ASN

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Mol	Chain	Res	Type
3	F	2	TYR
1	G	11	SER
1	G	17	ARG
1	G	25	VAL
1	G	35	ARG
1	G	75	ARG
1	G	82	LEU
1	G	88	SER
1	G	89	GLU
1	G	111	ARG
1	G	132	SER
1	G	186	LYS
1	G	216	THR
1	G	247	VAL
2	H	31	HIS
2	H	70	PHE
2	H	75	LYS
2	H	83	ASN
3	I	5	LEU
1	J	11	SER
1	J	17	ARG
1	J	25	VAL
1	J	35	ARG
1	J	88	SER
1	J	89	GLU
1	J	132	SER
1	J	216	THR
1	J	247	VAL
2	K	17	ASN
2	K	31	HIS
2	K	70	PHE
2	K	83	ASN
3	L	2	TYR
3	L	3	ASN
3	L	5	LEU
1	M	11	SER
1	M	25	VAL
1	M	35	ARG
1	M	88	SER
1	M	89	GLU
1	M	132	SER
1	M	216	THR

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Mol	Chain	Res	Type
1	M	247	VAL
2	N	31	HIS
2	N	70	PHE
2	N	75	LYS
2	N	83	ASN
3	O	3	ASN
3	O	5	LEU
1	P	11	SER
1	P	25	VAL
1	P	35	ARG
1	P	88	SER
1	P	89	GLU
1	P	111	ARG
1	P	132	SER
1	P	186	LYS
1	P	216	THR
1	P	247	VAL
2	Q	31	HIS
2	Q	70	PHE
2	Q	83	ASN
3	R	3	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	72	GLN
1	A	86	ASN
1	A	93	HIS
1	A	114	HIS
1	A	174	ASN
1	A	218	GLN
1	A	242	GLN
2	B	83	ASN
1	D	43	GLN
1	D	72	GLN
1	D	86	ASN
1	D	93	HIS
1	D	114	HIS
1	D	115	GLN
1	D	155	GLN
1	D	174	ASN

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Mol	Chain	Res	Type
1	D	218	GLN
1	D	242	GLN
2	E	31	HIS
2	E	83	ASN
3	F	1	ASN
3	F	3	ASN
1	G	43	GLN
1	G	86	ASN
1	G	93	HIS
1	G	114	HIS
1	G	115	GLN
1	G	155	GLN
1	G	174	ASN
1	G	197	HIS
1	G	218	GLN
1	G	242	GLN
2	H	31	HIS
2	H	83	ASN
2	H	89	GLN
3	I	1	ASN
3	I	3	ASN
1	J	43	GLN
1	J	86	ASN
1	J	93	HIS
1	J	114	HIS
1	J	115	GLN
1	J	174	ASN
1	J	218	GLN
1	J	242	GLN
2	K	31	HIS
2	K	83	ASN
3	L	1	ASN
3	L	3	ASN
1	M	43	GLN
1	M	86	ASN
1	M	93	HIS
1	M	114	HIS
1	M	115	GLN
1	M	155	GLN
1	M	174	ASN
1	M	218	GLN
1	M	242	GLN

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Mol	Chain	Res	Type
2	N	31	HIS
2	N	83	ASN
2	N	89	GLN
3	O	3	ASN
1	P	43	GLN
1	P	86	ASN
1	P	93	HIS
1	P	114	HIS
1	P	155	GLN
1	P	174	ASN
1	P	218	GLN
1	P	242	GLN
2	Q	31	HIS
2	Q	83	ASN
3	R	3	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)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	276/276 (100%)	0.15	10 (3%) 46 40	24, 62, 124, 182	0
1	D	276/276 (100%)	0.18	4 (1%) 73 68	30, 68, 115, 146	0
1	G	276/276 (100%)	0.24	8 (2%) 54 48	32, 69, 120, 140	0
1	J	276/276 (100%)	0.15	9 (3%) 49 43	28, 64, 125, 158	0
1	M	276/276 (100%)	0.20	6 (2%) 62 57	30, 68, 116, 134	0
1	P	276/276 (100%)	0.10	5 (1%) 67 62	25, 62, 124, 147	0
2	B	100/100 (100%)	0.19	2 (2%) 64 59	27, 62, 105, 123	0
2	E	100/100 (100%)	0.19	0 100 100	32, 65, 122, 127	0
2	H	100/100 (100%)	-0.03	0 100 100	30, 58, 93, 107	0
2	K	100/100 (100%)	0.15	0 100 100	30, 65, 129, 141	0
2	N	100/100 (100%)	-0.19	0 100 100	28, 53, 82, 97	0
2	Q	100/100 (100%)	0.05	0 100 100	27, 61, 104, 122	0
3	C	9/9 (100%)	0.36	0 100 100	33, 47, 63, 72	0
3	F	9/9 (100%)	0.19	1 (11%) 12 9	34, 53, 75, 77	0
3	I	9/9 (100%)	0.71	1 (11%) 12 9	42, 75, 86, 90	0
3	L	9/9 (100%)	-0.07	0 100 100	35, 51, 72, 75	0
3	O	9/9 (100%)	0.14	0 100 100	41, 67, 85, 88	0
3	R	9/9 (100%)	-0.06	0 100 100	33, 46, 62, 65	0
All	All	2310/2310 (100%)	0.14	46 (1%) 64 59	24, 64, 118, 182	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250	PRO	3.5
1	A	225	THR	3.4
2	B	99	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	M	16	GLY	3.3
1	A	249	VAL	3.1
1	G	40	ALA	3.1
1	A	274	TRP	2.9
3	I	6	PHE	2.9
1	M	40	ALA	2.9
1	J	16	GLY	2.8
1	G	57	PRO	2.8
1	D	16	GLY	2.7
1	A	197	HIS	2.7
1	P	255	GLN	2.5
3	F	4	TYR	2.4
1	G	41	ALA	2.3
1	G	18	GLY	2.3
1	A	259	CYS	2.3
1	G	20	PRO	2.3
1	A	248	VAL	2.3
1	G	16	GLY	2.3
1	M	17	ARG	2.2
1	J	193	PRO	2.2
1	J	249	VAL	2.2
1	P	108	ARG	2.2
1	P	248	VAL	2.2
1	J	154	GLU	2.2
1	G	75	ARG	2.2
1	J	1	GLY	2.2
1	A	190	THR	2.2
1	J	187	THR	2.2
1	G	59	TYR	2.2
1	J	248	VAL	2.2
1	J	17	ARG	2.2
1	M	195	SER	2.1
1	M	255	GLN	2.1
2	B	46	ILE	2.1
1	M	41	ALA	2.1
1	P	155	GLN	2.1
1	D	276	PRO	2.1
1	J	138	MET	2.1
1	D	41	ALA	2.1
1	A	276	PRO	2.0
1	P	154	GLU	2.0
1	A	272	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	17	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.