Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:02 PM GMT

PDB ID	:	1RQF
Title	:	Structure of CK2 beta subunit crystallized in the presence of a p21WAF1 peptide
Authors	:	Bertrand, L.; Sayed, M.F.; Pei, X.-Y.; Parisini, E.; Dhanaraj, V.; Bolanos-Garcia, V.M.; Allende, J.E.; Blundell, T.L.
Deposited on	:	2003-12-05
Resolution	:	2.89 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

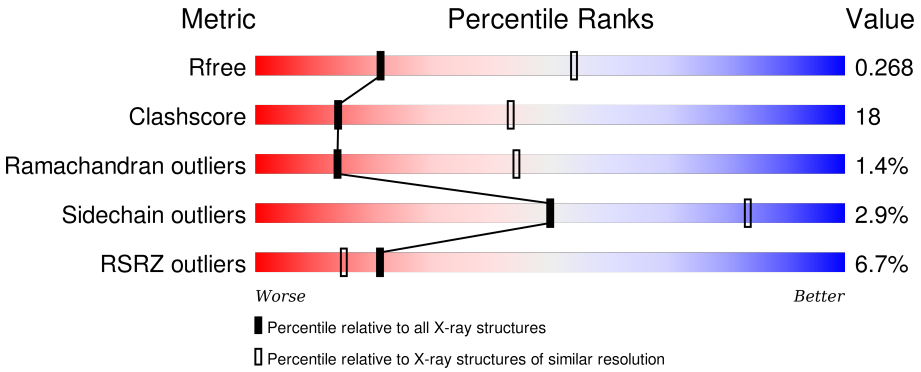
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.89 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	184	5% 65% 26% • 7%
1	B	184	4% 65% 22% • 10%
1	D	184	9% 63% 24% • 10%
1	E	184	5% 65% 27% • 6%
1	G	184	10% 62% 26% •• 10%

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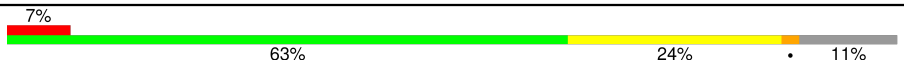
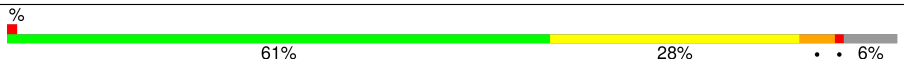
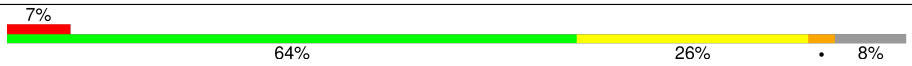
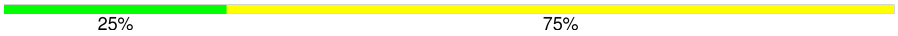
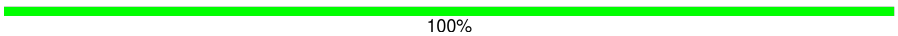
Mol	Chain	Length	Quality of chain
1	H	184	
1	J	184	
1	K	184	
2	M	4	
2	N	4	
2	T	4	
3	O	8	
4	P	3	
4	S	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ZN	D	201	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11216 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 Casein kinase II beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	172	Total	C	N	O	S	0	0	0
			1407	896	234	263	14			
1	B	165	Total	C	N	O	S	0	0	0
			1350	863	226	247	14			
1	D	165	Total	C	N	O	S	0	0	0
			1345	862	223	246	14			
1	E	173	Total	C	N	O	S	0	0	0
			1416	901	235	266	14			
1	G	165	Total	C	N	O	S	0	0	0
			1351	864	225	248	14			
1	H	163	Total	C	N	O	S	0	0	0
			1333	854	223	242	14			
1	J	173	Total	C	N	O	S	0	0	0
			1416	901	235	266	14			
1	K	169	Total	C	N	O	S	0	0	0
			1377	877	230	256	14			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	CLONING ARTIFACT	UNP P28021
A	-4	SER	-	CLONING ARTIFACT	UNP P28021
A	-3	PRO	-	CLONING ARTIFACT	UNP P28021
A	-2	GLY	-	CLONING ARTIFACT	UNP P28021
A	-1	ILE	-	CLONING ARTIFACT	UNP P28021
A	0	GLN	-	CLONING ARTIFACT	UNP P28021
B	-5	GLY	-	CLONING ARTIFACT	UNP P28021
B	-4	SER	-	CLONING ARTIFACT	UNP P28021
B	-3	PRO	-	CLONING ARTIFACT	UNP P28021
B	-2	GLY	-	CLONING ARTIFACT	UNP P28021
B	-1	ILE	-	CLONING ARTIFACT	UNP P28021
B	0	GLN	-	CLONING ARTIFACT	UNP P28021
D	-5	GLY	-	CLONING ARTIFACT	UNP P28021

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	SER	-	CLONING ARTIFACT	UNP P28021
D	-3	PRO	-	CLONING ARTIFACT	UNP P28021
D	-2	GLY	-	CLONING ARTIFACT	UNP P28021
D	-1	ILE	-	CLONING ARTIFACT	UNP P28021
D	0	GLN	-	CLONING ARTIFACT	UNP P28021
E	-5	GLY	-	CLONING ARTIFACT	UNP P28021
E	-4	SER	-	CLONING ARTIFACT	UNP P28021
E	-3	PRO	-	CLONING ARTIFACT	UNP P28021
E	-2	GLY	-	CLONING ARTIFACT	UNP P28021
E	-1	ILE	-	CLONING ARTIFACT	UNP P28021
E	0	GLN	-	CLONING ARTIFACT	UNP P28021
G	-5	GLY	-	CLONING ARTIFACT	UNP P28021
G	-4	SER	-	CLONING ARTIFACT	UNP P28021
G	-3	PRO	-	CLONING ARTIFACT	UNP P28021
G	-2	GLY	-	CLONING ARTIFACT	UNP P28021
G	-1	ILE	-	CLONING ARTIFACT	UNP P28021
G	0	GLN	-	CLONING ARTIFACT	UNP P28021
H	-5	GLY	-	CLONING ARTIFACT	UNP P28021
H	-4	SER	-	CLONING ARTIFACT	UNP P28021
H	-3	PRO	-	CLONING ARTIFACT	UNP P28021
H	-2	GLY	-	CLONING ARTIFACT	UNP P28021
H	-1	ILE	-	CLONING ARTIFACT	UNP P28021
H	0	GLN	-	CLONING ARTIFACT	UNP P28021
J	-5	GLY	-	CLONING ARTIFACT	UNP P28021
J	-4	SER	-	CLONING ARTIFACT	UNP P28021
J	-3	PRO	-	CLONING ARTIFACT	UNP P28021
J	-2	GLY	-	CLONING ARTIFACT	UNP P28021
J	-1	ILE	-	CLONING ARTIFACT	UNP P28021
J	0	GLN	-	CLONING ARTIFACT	UNP P28021
K	-5	GLY	-	CLONING ARTIFACT	UNP P28021
K	-4	SER	-	CLONING ARTIFACT	UNP P28021
K	-3	PRO	-	CLONING ARTIFACT	UNP P28021
K	-2	GLY	-	CLONING ARTIFACT	UNP P28021
K	-1	ILE	-	CLONING ARTIFACT	UNP P28021
K	0	GLN	-	CLONING ARTIFACT	UNP P28021

- Molecule 2 is a protein called Disordered segment of Cyclin-dependent kinase inhibitor 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	4	Total	C	N	O	0	0	0
			21	12	4	5			
2	N	4	Total	C	N	O	0	0	0
			21	12	4	5			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	T	4	Total C N O 21 12 4 5	0	0	0

- Molecule 3 is a protein called Disordered segment of Cyclin-dependent kinase inhibitor 1.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	O	8	Total C N O 41 24 8 9	0	0	0

- Molecule 4 is a protein called Disordered segment of Cyclin-dependent kinase inhibitor 1.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	P	3	Total C N O 16 9 3 4	0	0	0
4	S	3	Total C N O 16 9 3 4	0	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total Zn 1 1	0	0
5	J	1	Total Zn 1 1	0	0
5	D	1	Total Zn 1 1	0	0
5	K	1	Total Zn 1 1	0	0
5	E	1	Total Zn 1 1	0	0
5	H	1	Total Zn 1 1	0	0
5	B	1	Total Zn 1 1	0	0
5	A	1	Total Zn 1 1	0	0

- Molecule 6 is UNKNOWN (three-letter code: UNK) (formula: $C_4H_9NO_2$).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total C N O 6 3 1 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	E	1	Total	C	N	O	0	0
			6	3	1	2		

- Molecule 7 is water.

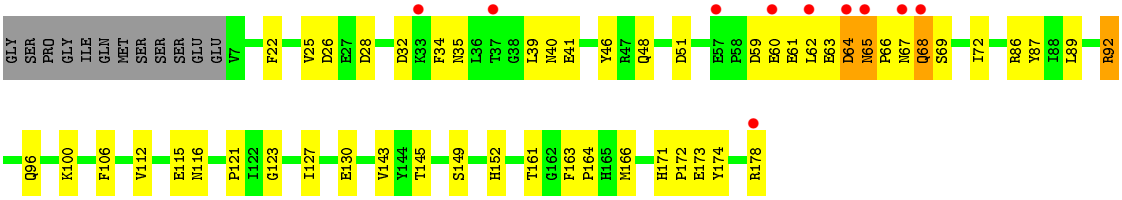
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	9	Total	O	0	0
			9	9		
7	B	7	Total	O	0	0
			7	7		
7	D	10	Total	O	0	0
			10	10		
7	E	7	Total	O	0	0
			7	7		
7	G	10	Total	O	0	0
			10	10		
7	H	7	Total	O	0	0
			7	7		
7	J	10	Total	O	0	0
			10	10		
7	K	3	Total	O	0	0
			3	3		
7	M	2	Total	O	0	0
			2	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

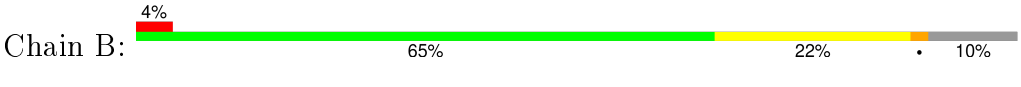
- Molecule 1: Casein kinase II beta chain

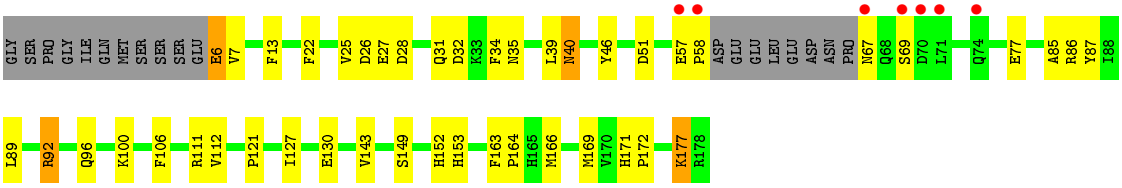
Chain A:



- Molecule 1: Casein kinase II beta chain

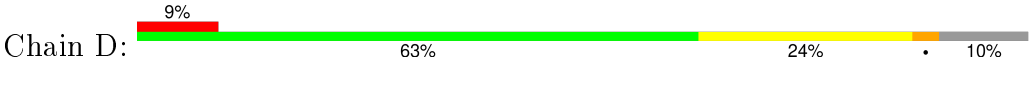
Chain B:

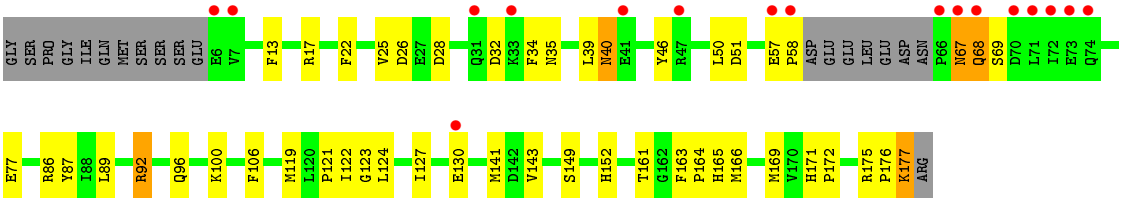




- Molecule 1: Casein kinase II beta chain

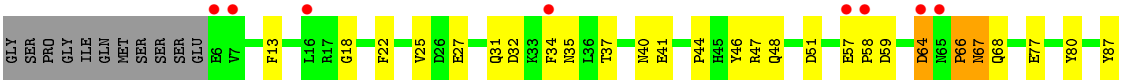
Chain D:





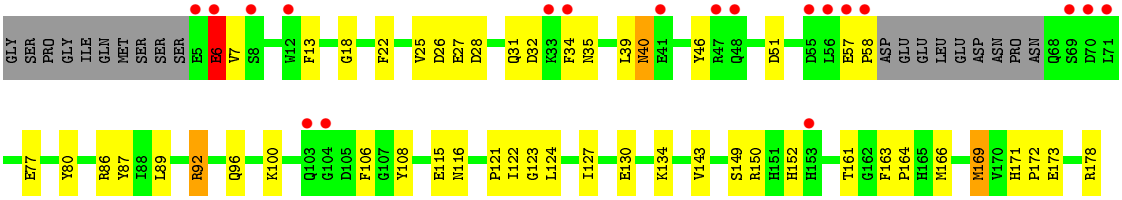
- Molecule 1: Casein kinase II beta chain

Chain E:



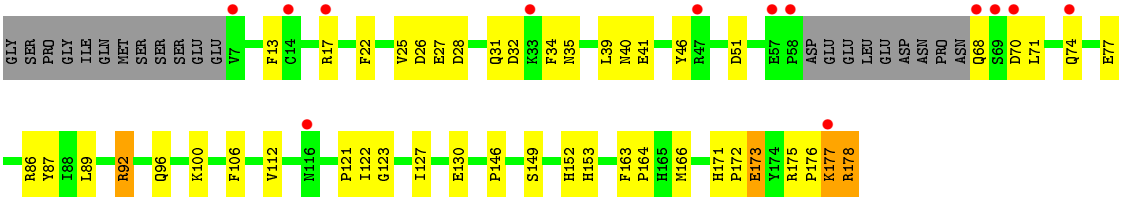
• Molecule 1: Casein kinase II beta chain

Chain G:



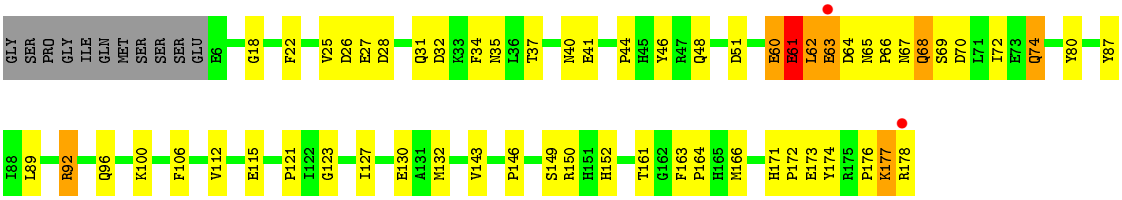
• Molecule 1: Casein kinase II beta chain

Chain H:



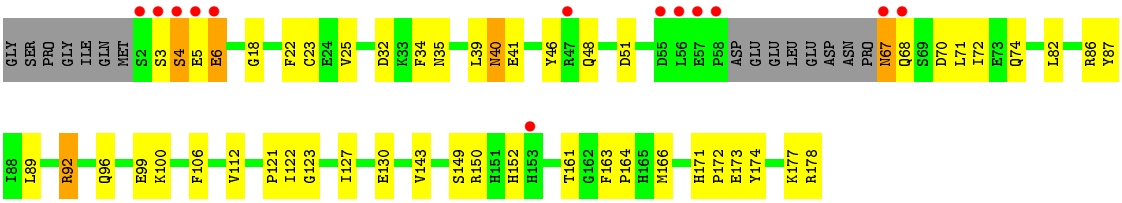
• Molecule 1: Casein kinase II beta chain

Chain J:



• Molecule 1: Casein kinase II beta chain

Chain K:



• Molecule 2: Disordered segment of Cyclin-dependent kinase inhibitor 1

Chain M:

• Molecule 2: Disordered segment of Cyclin-dependent kinase inhibitor 1

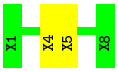
Chain N:

• Molecule 2: Disordered segment of Cyclin-dependent kinase inhibitor 1

Chain T:

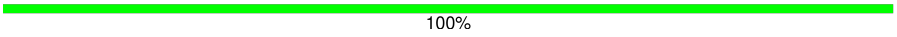
• Molecule 3: Disordered segment of Cyclin-dependent kinase inhibitor 1

Chain O:



• Molecule 4: Disordered segment of Cyclin-dependent kinase inhibitor 1

Chain P:



There are no outlier residues recorded for this chain.

• Molecule 4: Disordered segment of Cyclin-dependent kinase inhibitor 1

Chain S:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	145.42Å 170.63Å 74.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	11.97 – 2.89 11.97 – 2.89	Depositor EDS
% Data completeness (in resolution range)	100.0 (11.97-2.89) 99.5 (11.97-2.89)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.04 (at 2.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.238 , 0.266 0.239 , 0.268	Depositor DCC
R_{free} test set	2048 reflections (4.99%)	DCC
Wilson B-factor (Å^2)	70.2	Xtriage
Anisotropy	0.716	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 89.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 41307 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11216	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.39	0/1448	0.57	0/1961
1	B	0.41	0/1389	0.57	0/1878
1	D	0.38	0/1385	0.56	0/1875
1	E	0.39	0/1457	0.56	0/1973
1	G	0.53	3/1390 (0.2%)	0.55	0/1879
1	H	0.39	0/1372	0.55	0/1855
1	J	0.42	0/1457	0.60	0/1973
1	K	0.39	0/1416	0.55	0/1914
All	All	0.41	3/11314 (0.0%)	0.56	0/15308

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	6	GLU	CD-OE1	8.69	1.35	1.25
1	G	6	GLU	CD-OE2	7.96	1.34	1.25
1	G	6	GLU	CB-CG	7.26	1.66	1.52

There are no bond angle outliers.

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	1407	0	1323	56	0
1	B	1350	0	1278	49	0
1	D	1345	0	1273	53	0
1	E	1416	0	1329	52	0
1	G	1351	0	1278	52	0
1	H	1333	0	1266	59	0
1	J	1416	0	1329	64	0
1	K	1377	0	1299	46	0
2	M	21	0	10	4	0
2	N	21	0	9	1	0
2	T	21	0	6	4	0
3	O	41	0	19	1	0
4	P	16	0	6	0	0
4	S	16	0	5	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
6	E	6	0	3	0	0
6	G	6	0	3	0	0
7	A	9	0	0	0	0
7	B	7	0	0	2	0
7	D	10	0	0	2	0
7	E	7	0	0	3	0
7	G	10	0	0	1	0
7	H	7	0	0	1	0
7	J	10	0	0	1	0
7	K	3	0	0	1	0
7	M	2	0	0	0	0
All	All	11216	0	10436	392	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 18.

All (392) 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:60:GLU:HG3	1:A:62:LEU:HD23	1.30	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:MET:HG3	1:D:175:ARG:HD2	1.46	0.97
1:B:177:LYS:HE3	1:B:177:LYS:H	1.31	0.95
1:G:6:GLU:HG2	1:G:7:VAL:HG22	1.46	0.95
1:B:152:HIS:CE1	1:J:41:GLU:HG3	2.01	0.95
1:E:41:GLU:HG3	1:H:152:HIS:CE1	2.05	0.91
1:J:40:ASN:HD22	1:J:46:TYR:HB2	1.35	0.90
1:B:152:HIS:ND1	1:J:41:GLU:HG3	1.85	0.90
1:K:40:ASN:HA	1:K:46:TYR:CD1	2.10	0.87
1:J:66:PRO:O	1:J:69:SER:HB3	1.74	0.86
1:A:63:GLU:HG3	1:A:64:ASP:H	1.42	0.82
1:H:17:ARG:HH11	1:J:67:ASN:HB2	1.45	0.82
1:E:41:GLU:HG3	1:H:152:HIS:ND1	1.93	0.82
1:J:40:ASN:HB3	1:J:46:TYR:CD2	2.15	0.82
1:A:63:GLU:CG	1:A:64:ASP:H	1.92	0.81
1:B:177:LYS:H	1:B:177:LYS:CE	1.95	0.80
1:H:173:GLU:CD	1:H:173:GLU:H	1.83	0.79
1:J:40:ASN:ND2	1:J:46:TYR:HB2	1.97	0.79
1:G:57:GLU:OE1	1:G:58:PRO:HD2	1.83	0.78
1:J:177:LYS:HD3	1:J:178:ARG:H	1.50	0.77
1:A:115:GLU:HG2	2:M:4:UNK:H2	1.49	0.77
1:B:85:ALA:HB1	2:M:1:UNK:N	1.99	0.76
1:J:74:GLN:HA	1:J:74:GLN:HE21	1.52	0.75
1:H:178:ARG:N	1:H:178:ARG:HD3	2.02	0.74
1:D:176:PRO:O	1:D:177:LYS:HB2	1.86	0.73
1:G:40:ASN:HA	1:G:46:TYR:CD1	2.23	0.73
1:J:22:PHE:O	1:J:100:LYS:HE3	1.89	0.73
1:A:60:GLU:HG3	1:A:62:LEU:CD2	2.15	0.72
1:J:177:LYS:CD	1:J:178:ARG:H	2.03	0.72
1:A:61:GLU:O	1:A:62:LEU:HD22	1.90	0.72
1:J:115:GLU:HA	4:S:1:UNK:H2	1.54	0.72
1:K:22:PHE:O	1:K:100:LYS:HE3	1.90	0.71
1:E:66:PRO:HG2	1:E:67:ASN:H	1.56	0.71
1:D:57:GLU:OE1	1:D:58:PRO:HD2	1.90	0.70
1:E:57:GLU:OE1	1:E:58:PRO:HD2	1.91	0.70
1:B:40:ASN:HA	1:B:46:TYR:CD1	2.27	0.70
1:H:40:ASN:HA	1:H:46:TYR:CD1	2.27	0.70
1:A:22:PHE:O	1:A:100:LYS:HE3	1.92	0.69
1:J:177:LYS:HD3	1:J:178:ARG:N	2.08	0.69
1:B:177:LYS:HE3	1:B:177:LYS:N	2.04	0.68
1:E:66:PRO:HG2	1:E:67:ASN:OD1	1.93	0.68
1:A:178:ARG:HD3	1:E:125:SER:CB	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:TYR:OH	1:B:92:ARG:HD2	1.92	0.68
1:J:143:VAL:HG12	1:K:112:VAL:HG21	1.76	0.68
1:G:87:TYR:OH	1:G:92:ARG:HD2	1.94	0.68
1:H:87:TYR:OH	1:H:92:ARG:HD2	1.93	0.68
1:A:40:ASN:HA	1:A:46:TYR:CD1	2.30	0.67
1:E:47:ARG:NE	1:G:115:GLU:OE1	2.28	0.67
1:A:178:ARG:HD3	1:E:125:SER:OG	1.94	0.67
1:H:13:PHE:HE1	1:H:77:GLU:HG3	1.60	0.67
1:A:63:GLU:HG3	1:A:64:ASP:N	2.10	0.67
1:H:175:ARG:HG2	1:H:177:LYS:HG2	1.76	0.67
1:A:87:TYR:OH	1:A:92:ARG:HD2	1.96	0.66
1:J:115:GLU:HA	4:S:1:UNK:N	2.10	0.66
1:J:87:TYR:OH	1:J:92:ARG:HD2	1.95	0.66
1:E:40:ASN:HB3	1:E:46:TYR:CD2	2.31	0.65
1:H:17:ARG:NH1	1:J:67:ASN:HB2	2.11	0.65
1:B:177:LYS:H	1:B:177:LYS:CD	2.09	0.64
1:H:175:ARG:HD3	1:H:177:LYS:NZ	2.12	0.64
1:E:87:TYR:OH	1:E:92:ARG:HD2	1.98	0.64
1:J:143:VAL:HG12	1:K:112:VAL:CG2	2.28	0.64
1:E:46:TYR:CE1	1:G:116:ASN:ND2	2.66	0.64
1:E:163:PHE:HB3	1:E:164:PRO:HD3	1.78	0.64
1:A:63:GLU:CG	1:A:64:ASP:N	2.61	0.63
1:H:171:HIS:HA	1:H:173:GLU:OE2	1.97	0.63
1:A:163:PHE:HB3	1:A:164:PRO:HD3	1.78	0.63
1:B:163:PHE:HB3	1:B:164:PRO:HD3	1.81	0.63
1:B:13:PHE:HE1	1:B:77:GLU:HG3	1.63	0.63
1:G:22:PHE:O	1:G:100:LYS:HE3	1.99	0.63
1:D:87:TYR:OH	1:D:92:ARG:HD2	1.98	0.63
1:D:163:PHE:HB3	1:D:164:PRO:HD3	1.81	0.62
1:D:172:PRO:HB3	1:D:175:ARG:NH2	2.14	0.62
1:J:74:GLN:HA	1:J:74:GLN:NE2	2.14	0.62
1:K:3:SER:O	1:K:4:SER:HB2	1.99	0.62
1:G:40:ASN:HA	1:G:46:TYR:CE1	2.36	0.61
1:H:13:PHE:CE1	1:H:77:GLU:HG3	2.35	0.61
1:G:163:PHE:HB3	1:G:164:PRO:HD3	1.83	0.61
1:K:87:TYR:OH	1:K:92:ARG:HD2	2.00	0.61
1:J:62:LEU:O	1:J:62:LEU:HD13	2.01	0.61
1:K:67:ASN:HD22	1:K:67:ASN:C	2.04	0.60
1:H:39:LEU:HG	1:H:86:ARG:CZ	2.30	0.60
1:E:77:GLU:HB2	7:E:206:HOH:O	2.00	0.60
1:A:64:ASP:O	1:A:65:ASN:C	2.39	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:TYR:HH	1:D:92:ARG:HD2	1.66	0.60
1:E:22:PHE:O	1:E:100:LYS:HE3	2.02	0.60
1:B:13:PHE:CE1	1:B:77:GLU:HG3	2.37	0.59
1:H:163:PHE:HB3	1:H:164:PRO:HD3	1.83	0.59
1:H:127:ILE:HB	1:H:130:GLU:CG	2.32	0.59
1:J:127:ILE:HB	1:J:130:GLU:CG	2.32	0.59
1:H:22:PHE:O	1:H:100:LYS:HE3	2.02	0.59
1:J:163:PHE:HB3	1:J:164:PRO:HD3	1.84	0.59
2:T:1:UNK:C	2:T:3:UNK:N	2.63	0.59
1:H:146:PRO:HD2	7:H:305:HOH:O	2.02	0.59
1:A:143:VAL:HG12	1:B:112:VAL:HG21	1.85	0.59
1:H:178:ARG:N	1:H:178:ARG:CD	2.65	0.59
1:E:67:ASN:HB3	7:G:310:HOH:O	2.02	0.58
1:J:48:GLN:OE1	1:J:72:ILE:HD11	2.01	0.58
1:G:127:ILE:HB	1:G:130:GLU:CG	2.33	0.58
1:K:127:ILE:HB	1:K:130:GLU:CG	2.33	0.58
1:A:127:ILE:HB	1:A:130:GLU:CG	2.33	0.58
1:K:48:GLN:OE1	1:K:72:ILE:HD11	2.04	0.58
1:G:87:TYR:OH	1:G:96:GLN:NE2	2.36	0.58
1:K:87:TYR:OH	1:K:96:GLN:NE2	2.37	0.58
1:E:13:PHE:HE1	1:E:77:GLU:HG3	1.69	0.57
1:E:13:PHE:CE1	1:E:77:GLU:HG3	2.38	0.57
1:D:127:ILE:HB	1:D:130:GLU:CG	2.34	0.57
1:D:143:VAL:HG12	1:E:112:VAL:HG21	1.85	0.57
1:A:116:ASN:HB3	1:J:44:PRO:HA	1.85	0.57
1:G:143:VAL:HG12	1:H:112:VAL:CG2	2.35	0.57
1:K:163:PHE:HB3	1:K:164:PRO:HD3	1.85	0.57
1:B:111:ARG:HH22	1:E:141:MET:CE	2.17	0.57
1:B:127:ILE:HB	1:B:130:GLU:CG	2.34	0.57
1:H:87:TYR:OH	1:H:96:GLN:NE2	2.37	0.57
1:H:127:ILE:HB	1:H:130:GLU:HG2	1.87	0.57
1:A:39:LEU:HG	1:A:86:ARG:CZ	2.35	0.57
1:E:47:ARG:HE	1:G:115:GLU:CD	2.07	0.57
1:D:22:PHE:O	1:D:100:LYS:HE3	2.05	0.57
1:D:87:TYR:OH	1:D:96:GLN:NE2	2.38	0.56
1:B:87:TYR:HH	1:B:92:ARG:HD2	1.69	0.56
1:E:127:ILE:HB	1:E:130:GLU:CG	2.35	0.56
1:J:87:TYR:OH	1:J:96:GLN:NE2	2.38	0.56
1:A:116:ASN:ND2	1:J:46:TYR:CE1	2.74	0.56
1:A:178:ARG:HD3	1:E:125:SER:HG	1.70	0.56
1:G:127:ILE:HB	1:G:130:GLU:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:66:PRO:O	1:J:70:ASP:OD1	2.23	0.56
1:B:153:HIS:HD2	1:J:37:THR:OG1	1.89	0.56
1:D:13:PHE:HE1	1:D:77:GLU:HG3	1.70	0.56
1:J:127:ILE:HB	1:J:130:GLU:HG2	1.88	0.55
1:G:143:VAL:HG12	1:H:112:VAL:HG21	1.88	0.55
1:H:87:TYR:HH	1:H:92:ARG:HD2	1.72	0.55
1:D:177:LYS:HZ3	1:D:177:LYS:HB2	1.70	0.55
1:E:87:TYR:OH	1:E:96:GLN:NE2	2.39	0.55
1:K:127:ILE:HB	1:K:130:GLU:HG2	1.89	0.55
1:D:39:LEU:HD21	1:D:86:ARG:HE	1.72	0.55
1:D:25:VAL:HA	1:D:87:TYR:CE2	2.42	0.55
1:J:178:ARG:HG2	1:J:178:ARG:OXT	2.06	0.55
1:B:127:ILE:HB	1:B:130:GLU:HG2	1.89	0.55
1:A:143:VAL:HG12	1:B:112:VAL:CG2	2.37	0.55
1:D:67:ASN:ND2	1:D:67:ASN:O	2.39	0.55
1:A:127:ILE:HB	1:A:130:GLU:HG2	1.87	0.54
3:O:4:UNK:O	3:O:5:UNK:C	2.54	0.54
1:B:57:GLU:OE1	1:B:58:PRO:HD2	2.07	0.54
1:G:39:LEU:HD21	1:G:86:ARG:HD2	1.89	0.54
1:B:153:HIS:CD2	1:J:37:THR:HB	2.42	0.54
1:D:13:PHE:CE1	1:D:77:GLU:HG3	2.42	0.54
1:A:115:GLU:HG2	2:M:4:UNK:N	2.18	0.54
1:G:169:MET:CE	1:G:169:MET:HA	2.37	0.54
1:G:89:LEU:HD22	1:G:166:MET:HG3	1.89	0.54
1:A:92:ARG:HD3	1:A:92:ARG:O	2.07	0.54
1:A:40:ASN:OD1	1:A:41:GLU:OE2	2.26	0.54
2:M:1:UNK:O	2:M:2:UNK:C	2.54	0.54
1:D:39:LEU:HG	1:D:86:ARG:NH2	2.23	0.54
1:D:176:PRO:O	1:D:177:LYS:CB	2.56	0.54
1:H:92:ARG:HD3	1:H:92:ARG:O	2.08	0.54
1:J:89:LEU:HD22	1:J:166:MET:HG3	1.90	0.54
2:T:1:UNK:O	2:T:3:UNK:N	2.41	0.53
1:A:87:TYR:OH	1:A:96:GLN:NE2	2.40	0.53
1:J:32:ASP:HB3	1:J:35:ASN:ND2	2.24	0.53
1:H:89:LEU:HD22	1:H:166:MET:HG3	1.91	0.53
1:E:47:ARG:HB3	1:G:115:GLU:OE1	2.07	0.53
1:B:87:TYR:OH	1:B:96:GLN:NE2	2.42	0.53
1:G:150:ARG:NH2	1:J:60:GLU:OE2	2.41	0.53
1:G:6:GLU:HG3	1:G:7:VAL:HG13	1.91	0.53
1:E:25:VAL:HG23	1:E:80:TYR:OH	2.09	0.53
1:E:32:ASP:HB3	1:E:35:ASN:ND2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:176:PRO:O	1:J:177:LYS:O	2.27	0.52
1:D:39:LEU:CD2	1:D:86:ARG:HH21	2.21	0.52
1:B:32:ASP:HB3	1:B:35:ASN:ND2	2.24	0.52
1:D:127:ILE:HB	1:D:130:GLU:HG2	1.90	0.52
1:G:13:PHE:CE1	1:G:77:GLU:HG3	2.44	0.52
1:E:177:LYS:O	1:E:178:ARG:HB2	2.07	0.52
1:D:68:GLN:O	1:D:68:GLN:HG3	2.09	0.52
1:E:127:ILE:HB	1:E:130:GLU:HG2	1.91	0.52
1:K:5:GLU:HG2	1:K:6:GLU:N	2.25	0.52
1:G:124:LEU:HD11	1:H:112:VAL:HG11	1.90	0.52
1:B:149:SER:HA	1:B:152:HIS:CE1	2.45	0.52
1:E:89:LEU:HD22	1:E:166:MET:HG3	1.92	0.52
7:B:184:HOH:O	1:D:141:MET:CE	2.56	0.52
1:A:89:LEU:HD22	1:A:166:MET:HG3	1.92	0.52
1:J:65:ASN:ND2	1:J:68:GLN:HB2	2.25	0.52
1:B:92:ARG:HD3	1:B:92:ARG:O	2.11	0.51
1:J:74:GLN:CA	1:J:74:GLN:HE21	2.23	0.51
1:K:92:ARG:O	1:K:92:ARG:HD3	2.10	0.51
1:K:5:GLU:CG	1:K:6:GLU:N	2.74	0.51
1:E:18:GLY:HA2	1:E:150:ARG:HG3	1.92	0.51
1:B:89:LEU:HD22	1:B:166:MET:HG3	1.91	0.51
1:J:60:GLU:OE1	1:J:61:GLU:N	2.43	0.51
1:D:149:SER:HA	1:D:152:HIS:CE1	2.46	0.51
1:K:89:LEU:HD22	1:K:166:MET:HG3	1.93	0.51
1:D:166:MET:O	1:D:169:MET:HB2	2.10	0.51
1:G:92:ARG:O	1:G:92:ARG:HD3	2.11	0.51
1:H:175:ARG:HD3	1:H:177:LYS:HZ2	1.75	0.51
1:G:134:LYS:HD2	1:H:112:VAL:CG2	2.41	0.51
1:A:32:ASP:HB3	1:A:35:ASN:ND2	2.26	0.51
1:D:92:ARG:HD3	1:D:92:ARG:O	2.11	0.50
1:G:6:GLU:CG	1:G:7:VAL:N	2.74	0.50
1:D:89:LEU:HD22	1:D:166:MET:HG3	1.93	0.50
1:D:32:ASP:HB3	1:D:35:ASN:ND2	2.26	0.50
1:J:132:MET:HB2	2:T:1:UNK:CB	2.41	0.50
1:J:146:PRO:HA	7:J:406:HOH:O	2.11	0.50
1:G:13:PHE:HE1	1:G:77:GLU:HG3	1.76	0.50
1:J:18:GLY:HA2	1:J:150:ARG:HG3	1.93	0.50
1:E:154:THR:N	7:E:205:HOH:O	2.44	0.50
1:D:172:PRO:O	1:D:175:ARG:HB2	2.12	0.50
1:B:149:SER:HA	1:B:152:HIS:ND1	2.27	0.50
1:A:67:ASN:O	1:A:68:GLN:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:PHE:O	1:B:100:LYS:HE3	2.11	0.50
1:K:70:ASP:O	1:K:74:GLN:HG3	2.11	0.49
1:D:46:TYR:OH	1:D:50:LEU:HD22	2.11	0.49
1:H:92:ARG:HD3	1:H:92:ARG:C	2.33	0.49
1:H:32:ASP:HB3	1:H:35:ASN:ND2	2.28	0.49
1:A:116:ASN:ND2	1:J:46:TYR:CD1	2.67	0.49
1:B:153:HIS:CD2	1:J:37:THR:OG1	2.65	0.49
1:A:92:ARG:C	1:A:92:ARG:HD3	2.33	0.49
1:A:67:ASN:O	1:A:69:SER:N	2.46	0.49
1:B:92:ARG:C	1:B:92:ARG:HD3	2.33	0.48
1:B:39:LEU:HD21	1:B:86:ARG:HE	1.77	0.48
1:A:116:ASN:CB	1:J:44:PRO:HA	2.43	0.48
1:H:70:ASP:O	1:H:74:GLN:HG3	2.14	0.48
1:G:123:GLY:O	1:G:161:THR:HG22	2.13	0.48
1:B:177:LYS:HG2	1:B:177:LYS:O	2.13	0.48
1:D:25:VAL:HG13	1:D:87:TYR:CG	2.49	0.48
1:K:92:ARG:HD3	1:K:92:ARG:C	2.34	0.48
1:E:123:GLY:O	1:E:161:THR:HG22	2.14	0.48
1:A:173:GLU:HG2	1:A:174:TYR:CD1	2.48	0.48
1:A:87:TYR:HH	1:A:92:ARG:HD2	1.78	0.48
1:K:87:TYR:HH	1:K:92:ARG:HD2	1.76	0.48
1:A:48:GLN:OE1	1:A:72:ILE:HD11	2.13	0.48
1:G:32:ASP:HB3	1:G:35:ASN:ND2	2.29	0.48
1:H:106:PHE:CD1	1:H:121:PRO:HD3	2.49	0.48
1:G:149:SER:HA	1:G:152:HIS:CE1	2.48	0.48
1:J:92:ARG:HD3	1:J:92:ARG:O	2.14	0.48
1:B:153:HIS:CD2	1:J:37:THR:CB	2.97	0.48
1:E:149:SER:HA	1:E:152:HIS:CE1	2.48	0.48
1:H:149:SER:HA	1:H:152:HIS:CE1	2.48	0.48
1:D:149:SER:HA	1:D:152:HIS:ND1	2.28	0.48
1:G:39:LEU:HD11	1:G:86:ARG:CD	2.44	0.48
1:A:67:ASN:C	1:A:69:SER:N	2.64	0.48
1:K:106:PHE:CD1	1:K:121:PRO:HD3	2.48	0.48
1:J:25:VAL:HG23	1:J:80:TYR:OH	2.13	0.48
1:K:18:GLY:HA2	1:K:150:ARG:HG3	1.96	0.48
1:K:67:ASN:O	1:K:71:LEU:HG	2.13	0.48
1:G:6:GLU:HG2	1:G:7:VAL:N	2.29	0.47
1:K:40:ASN:HB2	1:K:46:TYR:CD2	2.49	0.47
1:B:40:ASN:HB2	1:B:46:TYR:CD2	2.49	0.47
1:J:171:HIS:N	1:J:172:PRO:HD3	2.30	0.47
1:E:92:ARG:C	1:E:92:ARG:HD3	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:39:LEU:HD22	1:K:82:LEU:HB3	1.95	0.47
1:H:149:SER:OG	1:J:64:ASP:OD2	2.31	0.47
1:A:32:ASP:OD1	1:A:34:PHE:HB3	2.15	0.47
1:B:171:HIS:N	1:B:172:PRO:HD3	2.29	0.47
1:E:171:HIS:N	1:E:172:PRO:HD3	2.29	0.47
1:E:37:THR:OG1	1:H:153:HIS:HD2	1.98	0.47
1:J:92:ARG:HD3	1:J:92:ARG:C	2.35	0.47
1:G:92:ARG:HD3	1:G:92:ARG:C	2.34	0.47
1:D:143:VAL:HG12	1:E:112:VAL:CG2	2.43	0.47
1:K:149:SER:HA	1:K:152:HIS:CE1	2.50	0.47
1:A:63:GLU:CD	1:A:64:ASP:H	2.19	0.47
1:H:171:HIS:N	1:H:172:PRO:HD3	2.30	0.47
1:K:32:ASP:HB3	1:K:35:ASN:ND2	2.29	0.47
1:D:67:ASN:C	1:D:69:SER:H	2.18	0.46
1:G:171:HIS:N	1:G:172:PRO:HD3	2.30	0.46
1:E:66:PRO:CG	1:E:67:ASN:H	2.27	0.46
1:J:127:ILE:HB	1:J:130:GLU:HG3	1.96	0.46
1:A:171:HIS:N	1:A:172:PRO:HD3	2.30	0.46
1:D:92:ARG:HD3	1:D:92:ARG:C	2.35	0.46
1:B:39:LEU:HG	1:B:86:ARG:NH2	2.30	0.46
1:D:124:LEU:HA	7:D:205:HOH:O	2.14	0.46
1:A:63:GLU:OE1	1:A:64:ASP:N	2.49	0.46
1:H:40:ASN:CG	1:H:41:GLU:OE2	2.54	0.46
1:B:127:ILE:HB	1:B:130:GLU:HG3	1.98	0.46
1:G:106:PHE:CD1	1:G:121:PRO:HD3	2.51	0.46
1:B:25:VAL:HA	1:B:87:TYR:CE2	2.50	0.46
1:K:127:ILE:HB	1:K:130:GLU:HG3	1.98	0.46
1:A:149:SER:HA	1:A:152:HIS:CE1	2.51	0.46
1:H:149:SER:HA	1:H:152:HIS:ND1	2.31	0.46
1:K:40:ASN:HB2	1:K:46:TYR:CE2	2.51	0.46
1:E:149:SER:HA	1:E:152:HIS:ND1	2.31	0.46
1:H:68:GLN:O	1:H:68:GLN:HG3	2.16	0.46
1:H:25:VAL:HA	1:H:87:TYR:CE2	2.52	0.45
7:B:184:HOH:O	1:D:141:MET:HE1	2.15	0.45
1:G:32:ASP:OD1	1:G:34:PHE:HB3	2.16	0.45
1:K:40:ASN:HA	1:K:46:TYR:CE1	2.52	0.45
1:K:25:VAL:HA	1:K:87:TYR:CE2	2.52	0.45
1:J:173:GLU:HG2	1:J:174:TYR:CD1	2.51	0.45
1:D:171:HIS:N	1:D:172:PRO:HD3	2.32	0.45
1:H:39:LEU:HG	1:H:86:ARG:NH2	2.32	0.45
1:D:127:ILE:HB	1:D:130:GLU:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:178:ARG:HG2	1:E:178:ARG:O	2.16	0.45
1:G:127:ILE:HB	1:G:130:GLU:HG3	1.98	0.45
1:D:40:ASN:HA	1:D:46:TYR:CD1	2.51	0.45
1:B:6:GLU:N	1:B:6:GLU:OE1	2.49	0.45
1:J:27:GLU:O	1:J:31:GLN:HG3	2.16	0.45
1:B:106:PHE:CD1	1:B:121:PRO:HD3	2.51	0.45
1:D:25:VAL:HG13	1:D:87:TYR:CD1	2.51	0.45
1:J:152:HIS:HA	2:T:1:UNK:CB	2.47	0.45
1:D:106:PHE:HB2	7:D:202:HOH:O	2.16	0.45
1:H:32:ASP:OD1	1:H:34:PHE:HB3	2.17	0.45
1:K:123:GLY:O	1:K:161:THR:HG22	2.17	0.45
1:H:127:ILE:HB	1:H:130:GLU:HG3	1.98	0.44
1:G:134:LYS:HD2	1:H:112:VAL:HG22	1.98	0.44
1:B:39:LEU:HG	1:B:86:ARG:CZ	2.47	0.44
1:G:149:SER:HA	1:G:152:HIS:ND1	2.32	0.44
1:E:44:PRO:HB3	1:G:108:TYR:CE2	2.52	0.44
1:B:111:ARG:HH22	1:E:141:MET:HE3	1.82	0.44
1:G:18:GLY:HA2	1:G:150:ARG:HG3	1.99	0.44
1:E:48:GLN:HG2	1:E:59:ASP:OD1	2.17	0.44
1:J:63:GLU:HB3	1:J:64:ASP:H	1.61	0.44
1:B:32:ASP:OD1	1:B:34:PHE:HB3	2.16	0.44
1:D:32:ASP:OD1	1:D:34:PHE:HB3	2.16	0.44
1:G:27:GLU:O	1:G:31:GLN:HG3	2.18	0.44
1:A:106:PHE:CD1	1:A:121:PRO:HD3	2.52	0.44
1:K:171:HIS:N	1:K:172:PRO:HD3	2.33	0.44
1:E:92:ARG:O	1:E:92:ARG:HD3	2.17	0.44
1:E:127:ILE:HB	1:E:130:GLU:HG3	1.99	0.44
1:K:40:ASN:OD1	1:K:41:GLU:CD	2.56	0.44
1:G:122:ILE:HG12	1:G:123:GLY:N	2.33	0.44
1:K:149:SER:HA	1:K:152:HIS:ND1	2.33	0.44
1:H:177:LYS:HD3	1:H:177:LYS:HA	1.69	0.44
1:K:32:ASP:OD1	1:K:34:PHE:HB3	2.17	0.44
1:D:123:GLY:O	1:D:161:THR:HG22	2.17	0.44
1:H:175:ARG:HD3	1:H:177:LYS:HZ1	1.83	0.43
1:J:106:PHE:CD1	1:J:121:PRO:HD3	2.52	0.43
1:H:25:VAL:HG13	1:H:87:TYR:CG	2.53	0.43
1:A:127:ILE:HB	1:A:130:GLU:HG3	1.99	0.43
1:K:39:LEU:HG	1:K:86:ARG:NH1	2.33	0.43
1:K:23:CYS:HB2	7:K:403:HOH:O	2.18	0.43
1:E:106:PHE:CD1	1:E:121:PRO:HD3	2.53	0.43
1:H:40:ASN:HB3	1:H:46:TYR:CZ	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:ASP:OD1	1:E:34:PHE:HB3	2.17	0.43
1:D:67:ASN:HD22	1:D:67:ASN:C	2.21	0.43
1:K:173:GLU:HG2	1:K:174:TYR:CD1	2.52	0.43
1:K:68:GLN:NE2	1:K:68:GLN:O	2.51	0.43
1:G:25:VAL:HG23	1:G:80:TYR:OH	2.18	0.43
1:J:67:ASN:C	1:J:69:SER:N	2.71	0.43
1:H:39:LEU:HD21	1:H:86:ARG:NE	2.34	0.43
1:J:32:ASP:OD1	1:J:34:PHE:HB3	2.19	0.43
1:H:68:GLN:NE2	1:H:71:LEU:HD12	2.34	0.43
1:H:27:GLU:O	1:H:31:GLN:HG3	2.18	0.43
1:A:67:ASN:C	1:A:69:SER:H	2.22	0.43
1:K:177:LYS:HB3	1:K:178:ARG:H	1.55	0.43
1:E:46:TYR:CD1	1:G:116:ASN:ND2	2.69	0.42
1:K:5:GLU:O	1:K:6:GLU:HB2	2.19	0.42
1:J:112:VAL:HG21	1:K:143:VAL:HG12	2.01	0.42
1:H:40:ASN:HB3	1:H:46:TYR:CE2	2.54	0.42
1:D:106:PHE:CD1	1:D:121:PRO:HD3	2.54	0.42
1:B:67:ASN:C	1:B:69:SER:H	2.22	0.42
1:J:40:ASN:HD22	1:J:46:TYR:CB	2.19	0.42
1:H:26:ASP:HB3	1:H:28:ASP:OD1	2.19	0.42
1:A:145:THR:HG21	2:N:3:UNK:CB	2.49	0.42
1:A:26:ASP:HB3	1:A:28:ASP:OD1	2.19	0.42
1:J:149:SER:HA	1:J:152:HIS:CE1	2.54	0.42
1:K:5:GLU:CG	1:K:6:GLU:H	2.33	0.42
1:B:172:PRO:HG2	1:D:165:HIS:HD2	1.84	0.42
1:H:26:ASP:OD2	1:H:92:ARG:NE	2.53	0.42
1:A:25:VAL:HA	1:A:87:TYR:CE2	2.55	0.42
1:E:27:GLU:O	1:E:31:GLN:HG3	2.20	0.42
1:A:65:ASN:O	1:A:66:PRO:C	2.57	0.42
1:G:40:ASN:ND2	1:G:46:TYR:CE2	2.88	0.42
1:J:26:ASP:HB3	1:J:28:ASP:OD1	2.20	0.42
7:E:208:HOH:O	1:G:173:GLU:HG3	2.19	0.42
1:J:149:SER:HA	1:J:152:HIS:ND1	2.35	0.41
1:A:112:VAL:HG21	1:B:143:VAL:HG12	2.02	0.41
1:G:26:ASP:HB3	1:G:28:ASP:OD1	2.20	0.41
1:H:25:VAL:HG13	1:H:87:TYR:CD1	2.55	0.41
1:A:123:GLY:O	1:A:161:THR:HG22	2.20	0.41
1:D:177:LYS:HB2	1:D:177:LYS:NZ	2.35	0.41
1:H:106:PHE:CG	1:H:121:PRO:HD3	2.56	0.41
1:G:173:GLU:CD	1:G:173:GLU:H	2.24	0.41
1:D:26:ASP:HB3	1:D:28:ASP:OD1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:123:GLY:O	1:J:161:THR:HG22	2.20	0.41
1:A:61:GLU:C	1:A:62:LEU:HD22	2.40	0.41
1:G:40:ASN:HB3	1:G:46:TYR:CE2	2.56	0.41
1:D:39:LEU:HD23	1:D:86:ARG:HH21	1.86	0.41
1:A:64:ASP:O	1:A:66:PRO:N	2.53	0.41
1:H:39:LEU:HD21	1:H:86:ARG:HE	1.85	0.41
1:K:122:ILE:HG12	1:K:123:GLY:N	2.36	0.41
1:G:40:ASN:HA	1:G:46:TYR:CG	2.54	0.41
1:A:39:LEU:HG	1:A:86:ARG:NH2	2.36	0.41
1:A:149:SER:HA	1:A:152:HIS:ND1	2.35	0.41
1:B:27:GLU:O	1:B:31:GLN:HG3	2.20	0.41
1:K:96:GLN:O	1:K:99:GLU:HB3	2.21	0.41
1:G:7:VAL:O	1:G:7:VAL:HG23	2.21	0.40
1:D:67:ASN:O	1:D:69:SER:N	2.47	0.40
1:E:41:GLU:CD	1:E:41:GLU:H	2.25	0.40
1:E:122:ILE:HG12	1:E:123:GLY:N	2.36	0.40
1:K:106:PHE:CG	1:K:121:PRO:HD3	2.56	0.40
1:B:26:ASP:HB3	1:B:28:ASP:OD1	2.20	0.40
1:E:173:GLU:CD	1:E:173:GLU:H	2.24	0.40
1:H:122:ILE:HG12	1:H:123:GLY:N	2.36	0.40
1:D:106:PHE:HB2	1:D:119:MET:O	2.22	0.40
1:D:122:ILE:HG12	1:D:123:GLY:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	170/184 (92%)	161 (95%)	5 (3%)	4 (2%)	7 29
1	B	161/184 (88%)	155 (96%)	5 (3%)	1 (1%)	30 67
1	D	161/184 (88%)	156 (97%)	4 (2%)	1 (1%)	30 67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	171/184 (93%)	161 (94%)	6 (4%)	4 (2%)	8 30
1	G	161/184 (88%)	157 (98%)	3 (2%)	1 (1%)	30 67
1	H	159/184 (86%)	154 (97%)	3 (2%)	2 (1%)	15 46
1	J	171/184 (93%)	161 (94%)	6 (4%)	4 (2%)	8 30
1	K	165/184 (90%)	159 (96%)	4 (2%)	2 (1%)	16 48
All	All	1319/1472 (90%)	1264 (96%)	36 (3%)	19 (1%)	14 44

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	ASP
1	J	60	GLU
1	J	61	GLU
1	J	63	GLU
1	J	177	LYS
1	K	4	SER
1	B	7	VAL
1	E	64	ASP
1	A	64	ASP
1	A	68	GLN
1	D	68	GLN
1	E	66	PRO
1	E	67	ASN
1	E	68	GLN
1	H	177	LYS
1	G	6	GLU
1	K	6	GLU
1	A	65	ASN
1	H	176	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	153/163 (94%)	151 (99%)	2 (1%)	76 94
1	B	146/163 (90%)	141 (97%)	5 (3%)	44 79
1	D	146/163 (90%)	140 (96%)	6 (4%)	37 73
1	E	154/163 (94%)	151 (98%)	3 (2%)	65 89
1	G	146/163 (90%)	141 (97%)	5 (3%)	44 79
1	H	144/163 (88%)	140 (97%)	4 (3%)	51 84
1	J	154/163 (94%)	148 (96%)	6 (4%)	39 75
1	K	150/163 (92%)	146 (97%)	4 (3%)	52 84
All	All	1193/1304 (92%)	1158 (97%)	35 (3%)	50 83

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ASP
1	A	92	ARG
1	B	6	GLU
1	B	40	ASN
1	B	51	ASP
1	B	92	ARG
1	B	177	LYS
1	D	17	ARG
1	D	40	ASN
1	D	51	ASP
1	D	67	ASN
1	D	92	ARG
1	D	177	LYS
1	E	51	ASP
1	E	64	ASP
1	E	92	ARG
1	G	40	ASN
1	G	51	ASP
1	G	92	ARG
1	G	169	MET
1	G	178	ARG
1	H	51	ASP
1	H	92	ARG
1	H	173	GLU
1	H	178	ARG
1	J	51	ASP
1	J	61	GLU

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Mol	Chain	Res	Type
1	J	62	LEU
1	J	68	GLN
1	J	74	GLN
1	J	92	ARG
1	K	40	ASN
1	K	51	ASP
1	K	67	ASN
1	K	92	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	96	GLN
1	B	68	GLN
1	B	96	GLN
1	B	153	HIS
1	D	68	GLN
1	D	74	GLN
1	D	96	GLN
1	E	74	GLN
1	E	96	GLN
1	G	74	GLN
1	G	96	GLN
1	H	68	GLN
1	H	74	GLN
1	H	96	GLN
1	H	153	HIS
1	J	40	ASN
1	J	68	GLN
1	J	74	GLN
1	J	96	GLN
1	K	40	ASN
1	K	67	ASN
1	K	68	GLN
1	K	74	GLN
1	K	96	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 2 are unknown and 8 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	172/184 (93%)	0.17	10 (5%) 26 20	37, 72, 138, 182	7 (4%)
1	B	165/184 (89%)	0.02	7 (4%) 40 33	31, 63, 115, 155	4 (2%)
1	D	165/184 (89%)	0.37	17 (10%) 9 5	40, 79, 138, 187	4 (2%)
1	E	173/184 (94%)	0.14	9 (5%) 31 24	39, 66, 127, 168	4 (2%)
1	G	165/184 (89%)	0.62	19 (11%) 6 4	36, 94, 163, 190	9 (5%)
1	H	163/184 (88%)	0.24	13 (7%) 15 10	32, 71, 132, 166	4 (2%)
1	J	173/184 (94%)	-0.12	2 (1%) 81 78	38, 62, 115, 162	4 (2%)
1	K	169/184 (91%)	0.21	13 (7%) 16 11	8, 71, 125, 182	10 (5%)
2	M	0/4	-	-	-	-
2	N	0/4	-	-	-	-
2	T	0/4	-	-	-	-
3	O	0/8	-	-	-	-
4	P	0/3	-	-	-	-
4	S	0/3	-	-	-	-
All	All	1345/1498 (89%)	0.20	90 (6%) 21 15	8, 71, 138, 190	46 (3%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	58	PRO	7.9
1	K	58	PRO	6.6
1	A	62	LEU	6.0
1	K	68	GLN	5.9
1	G	34	PHE	5.9
1	G	57	GLU	5.8
1	H	69	SER	5.6
1	D	33	LYS	5.1
1	G	58	PRO	4.7
1	E	57	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	33	LYS	4.7
1	G	56	LEU	4.6
1	G	70	ASP	4.3
1	B	70	ASP	4.1
1	G	5	GLU	4.1
1	K	67	ASN	4.0
1	E	64	ASP	4.0
1	H	70	ASP	4.0
1	D	70	ASP	3.9
1	B	69	SER	3.9
1	K	57	GLU	3.8
1	D	67	ASN	3.8
1	A	65	ASN	3.7
1	D	66	PRO	3.6
1	E	6	GLU	3.6
1	H	33	LYS	3.5
1	H	74	GLN	3.5
1	G	69	SER	3.4
1	K	5	GLU	3.3
1	A	64	ASP	3.3
1	K	6	GLU	3.2
1	G	103	GLN	3.2
1	E	58	PRO	3.2
1	B	58	PRO	3.1
1	K	56	LEU	3.1
1	G	48	GLN	3.0
1	A	67	ASN	2.9
1	D	47	ARG	2.9
1	G	6	GLU	2.9
1	D	7	VAL	2.9
1	D	6	GLU	2.8
1	D	74	GLN	2.8
1	D	58	PRO	2.8
1	K	3	SER	2.7
1	G	33	LYS	2.7
1	D	68	GLN	2.7
1	E	178	ARG	2.7
1	H	57	GLU	2.6
1	B	67	ASN	2.5
1	G	55	ASP	2.5
1	D	72	ILE	2.5
1	A	57	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	47	ARG	2.4
1	E	16	LEU	2.4
1	J	63	GLU	2.4
1	K	55	ASP	2.4
1	B	71	LEU	2.3
1	D	130	GLU	2.3
1	H	7	VAL	2.3
1	A	60	GLU	2.3
1	D	57	GLU	2.3
1	D	73	GLU	2.3
1	D	31	GLN	2.3
1	A	178	ARG	2.3
1	G	153	HIS	2.3
1	D	41	GLU	2.3
1	G	8	SER	2.3
1	J	178	ARG	2.3
1	K	2	SER	2.3
1	K	153	HIS	2.2
1	G	41	GLU	2.2
1	H	116	ASN	2.2
1	E	34	PHE	2.2
1	E	65	ASN	2.2
1	H	47	ARG	2.2
1	E	7	VAL	2.2
1	G	12	TRP	2.2
1	K	4	SER	2.1
1	G	104	GLY	2.1
1	H	17	ARG	2.1
1	H	68	GLN	2.1
1	G	71	LEU	2.1
1	H	14	CYS	2.1
1	A	68	GLN	2.1
1	D	71	LEU	2.1
1	K	47	ARG	2.1
1	H	177	LYS	2.0
1	B	74	GLN	2.0
1	A	37	THR	2.0
1	B	57	GLU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	ZN	D	201	1/1	0.97	0.23	2.09	94,94,94,94	0
5	ZN	E	202	1/1	0.97	0.22	1.72	100,100,100,100	0
5	ZN	A	179	1/1	0.97	0.22	1.26	99,99,99,99	0
5	ZN	K	402	1/1	0.96	0.22	1.24	99,99,99,99	0
5	ZN	B	179	1/1	0.98	0.22	0.88	99,99,99,99	0
5	ZN	H	302	1/1	0.97	0.21	0.72	102,102,102,102	0
5	ZN	J	401	1/1	0.95	0.22	0.61	107,107,107,107	0
5	ZN	G	301	1/1	0.92	0.20	0.11	106,106,106,106	0
6	UNK	G	302	6/-	0.64	0.47	-	107,147,148,148	0
6	UNK	E	203	6/-	0.66	0.38	-	67,133,133,133	0

6.5 Other polymers (i)

There are no such residues in this entry.