Full wwPDB X-ray Structure Validation Report (i)

Sep 11, 2023 – 08:40 AM EDT

PDB ID	:	4MD9
Title	:	Crystal Structure of symmetric CK2 holoenzyme with mutated alpha subunit (F121E truncated at aa 336)
Authors	:	Lolli, G.; Ranchio, A.; Battistutta, R.
Deposited on	:	2013-08-22
Resolution	:	3.50 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 (i) 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 (1)) were used in the production of this report:

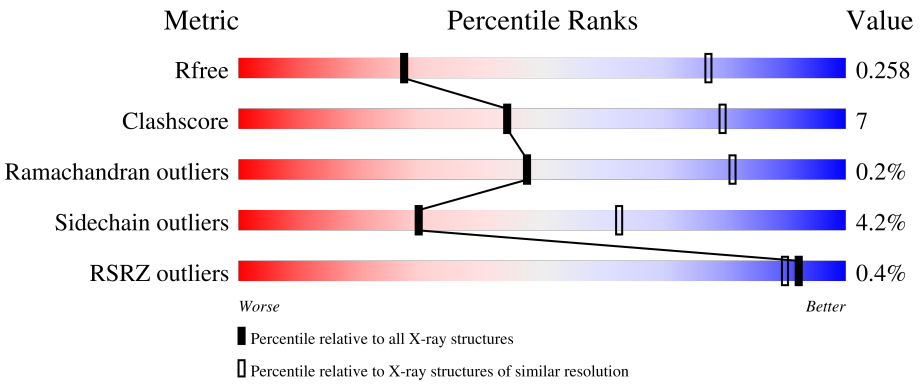
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.50 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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	215	78% 14% • 7%
1	B	215	81% 9% 9%
1	C	215	73% 18% • 8%
1	D	215	76% 14% 9%
1	I	215	76% 13% • 9%

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Mol	Chain	Length	Quality of chain
1	J	215	76% 13% • 10%
1	N	215	76% 13% • 8%
1	O	215	2% 77% 14% • 8%
2	E	336	% 81% 16% • •
2	F	336	% 84% 11% • •
2	G	336	79% 16% • •
2	H	336	85% 12% • •
2	K	336	% 82% 14% • •
2	L	336	88% 8% • •
2	M	336	78% 20% • •
2	P	336	85% 11% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 35073 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 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	201	1643	1053	275	300	15	0	0	0
1	B	195	1593	1025	268	285	15	0	0	0
1	C	198	1619	1039	271	294	15	0	0	0
1	D	196	1601	1029	270	287	15	0	0	0
1	I	196	1601	1029	269	288	15	0	0	0
1	J	194	1584	1020	267	282	15	0	0	0
1	N	197	1610	1034	270	291	15	0	0	0
1	O	198	1618	1038	272	293	15	0	0	0

- Molecule 2 is a protein called Casein kinase II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	329	2777	1777	488	501	11	0	0	0
2	F	327	2767	1772	486	498	11	0	0	0
2	G	329	2777	1777	488	501	11	0	0	0
2	H	328	2771	1774	487	499	11	0	0	0
2	K	328	2771	1774	487	499	11	0	0	0
2	L	328	2771	1774	487	499	11	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	331	2791	1785	491	504	11	0	0	0
			Total	C	N	O	S			
2	P	328	2771	1774	487	499	11	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	121	GLU	PHE	engineered mutation	UNP P68400
F	121	GLU	PHE	engineered mutation	UNP P68400
G	121	GLU	PHE	engineered mutation	UNP P68400
H	121	GLU	PHE	engineered mutation	UNP P68400
K	121	GLU	PHE	engineered mutation	UNP P68400
L	121	GLU	PHE	engineered mutation	UNP P68400
M	121	GLU	PHE	engineered mutation	UNP P68400
P	121	GLU	PHE	engineered mutation	UNP P68400

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

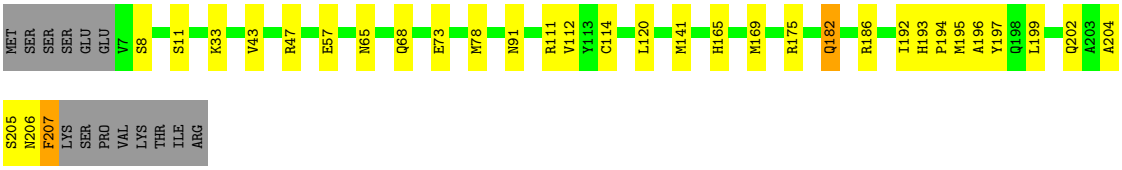
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0
			Total	Zn		
3	B	1	1	1	0	0
			Total	Zn		
3	C	1	1	1	0	0
			Total	Zn		
3	D	1	1	1	0	0
			Total	Zn		
3	I	1	1	1	0	0
			Total	Zn		
3	J	1	1	1	0	0
			Total	Zn		
3	N	1	1	1	0	0
			Total	Zn		
3	O	1	1	1	0	0

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: Casein kinase II subunit beta

Chain A:

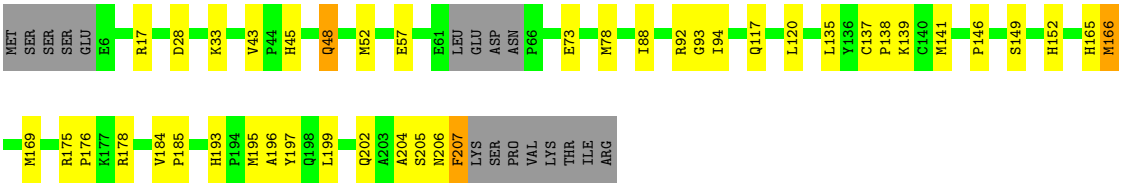


• Molecule 1: Casein kinase II subunit beta

Chain B:

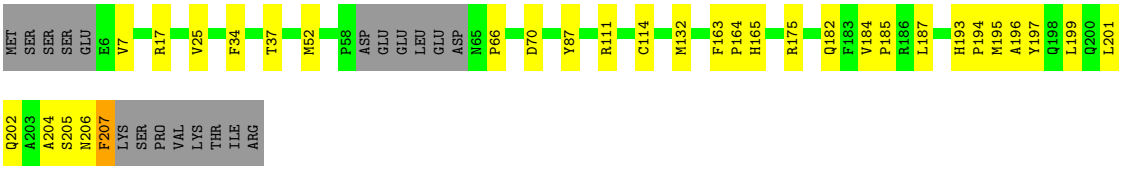
• Molecule 1: Casein kinase II subunit beta

Chain C:



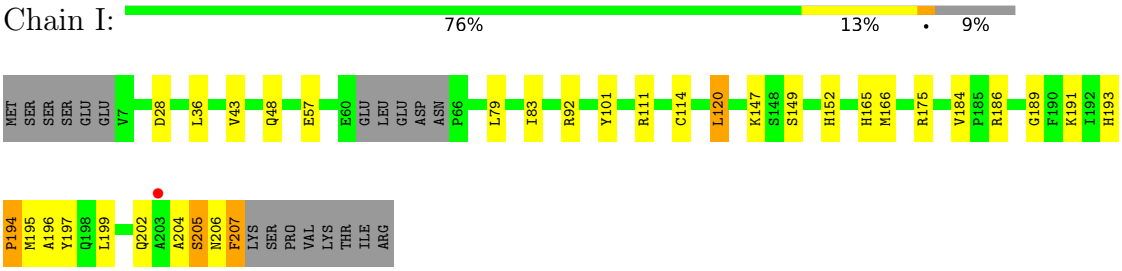
• Molecule 1: Casein kinase II subunit beta

Chain D:



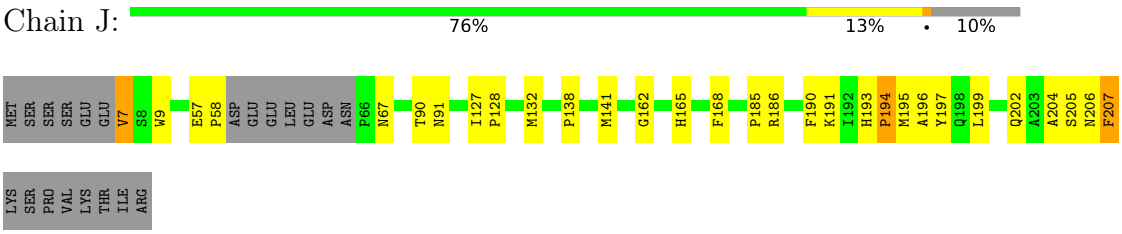
• Molecule 1: Casein kinase II subunit beta

Chain I:



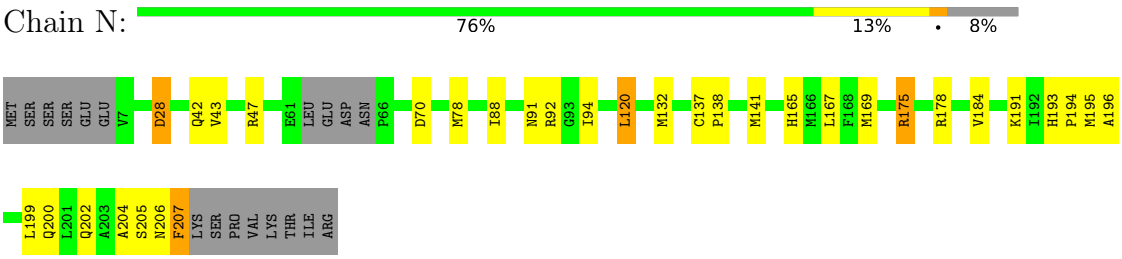
• Molecule 1: Casein kinase II subunit beta

Chain J:



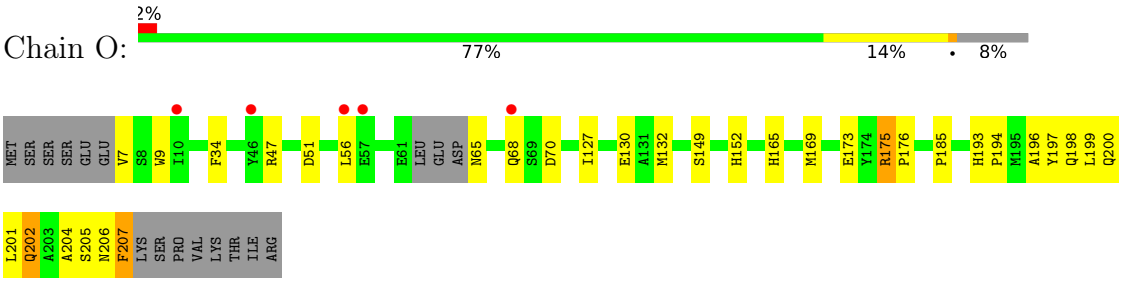
• Molecule 1: Casein kinase II subunit beta

Chain N:



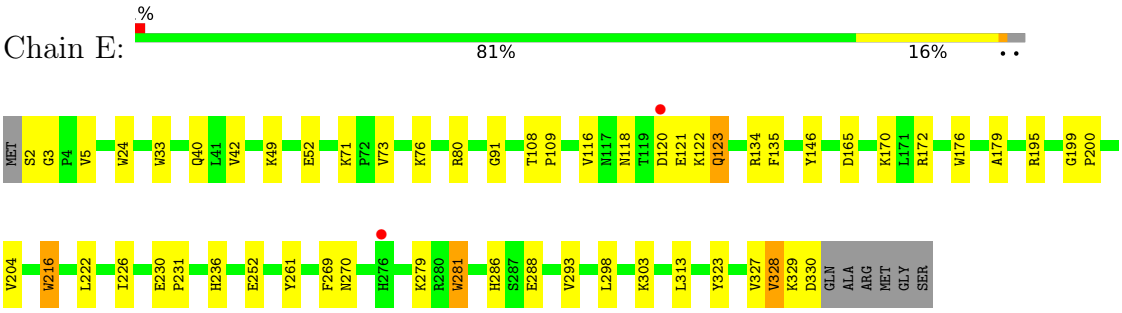
• Molecule 1: Casein kinase II subunit beta

Chain O:



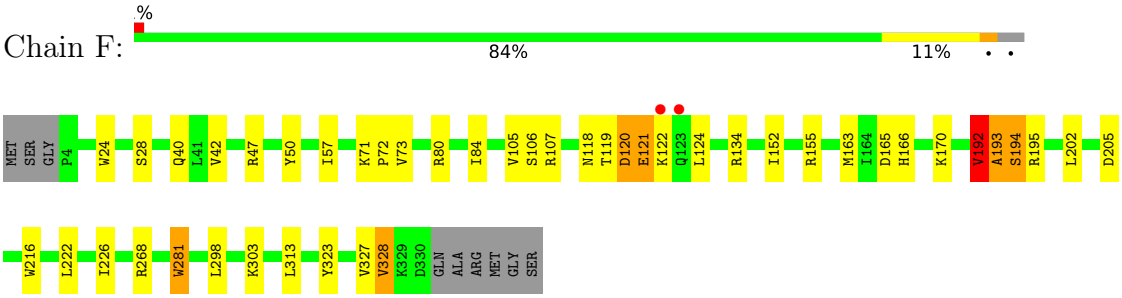
• Molecule 2: Casein kinase II subunit alpha

Chain E:



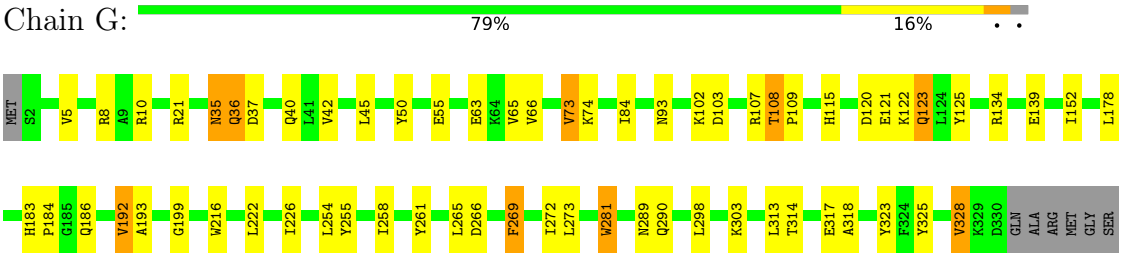
• Molecule 2: Casein kinase II subunit alpha

Chain F:



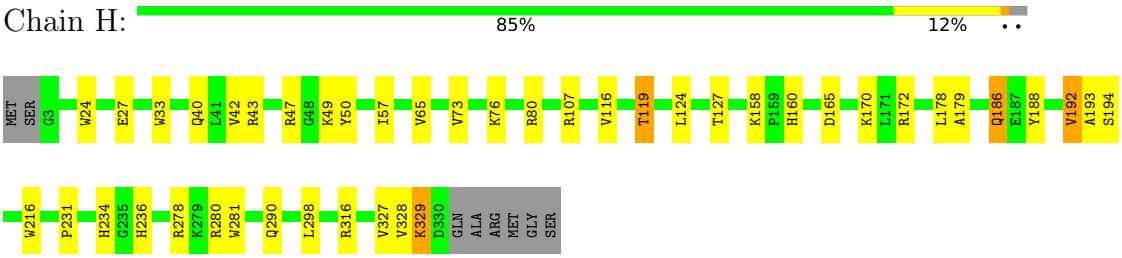
• Molecule 2: Casein kinase II subunit alpha

Chain G:



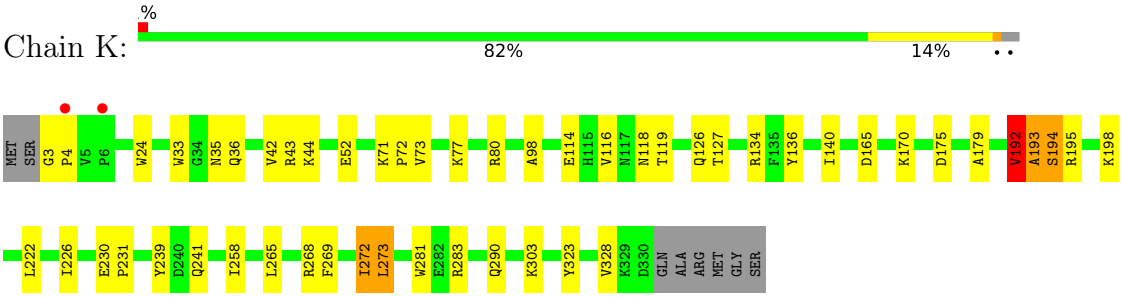
• Molecule 2: Casein kinase II subunit alpha

Chain H:



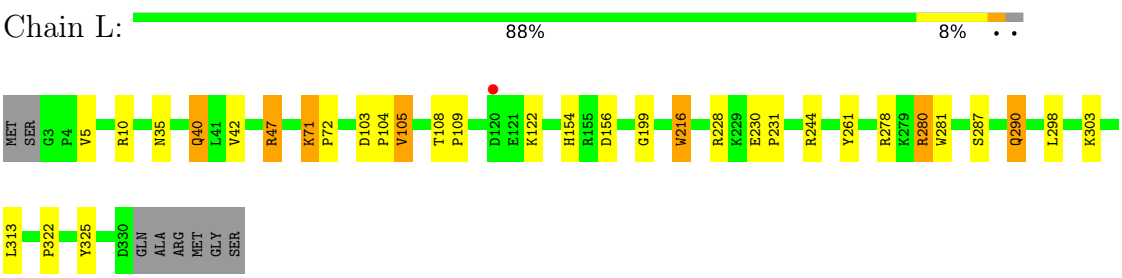
• Molecule 2: Casein kinase II subunit alpha

Chain K:



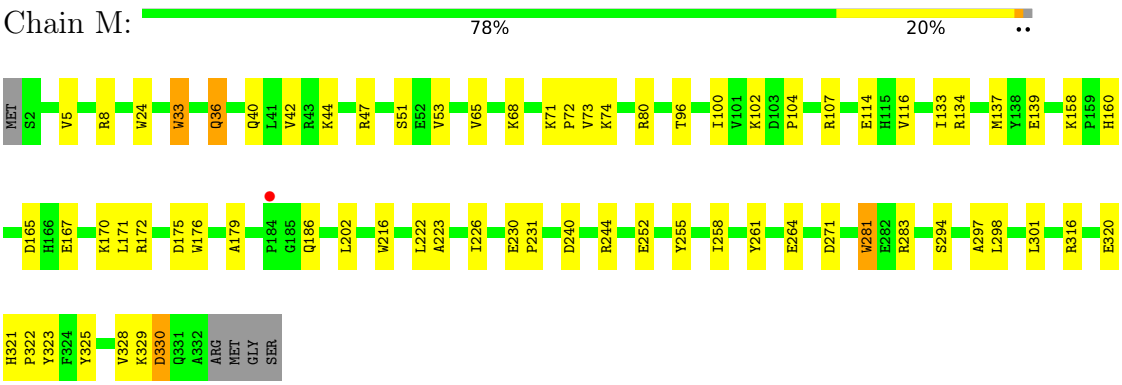
• Molecule 2: Casein kinase II subunit alpha

Chain L:



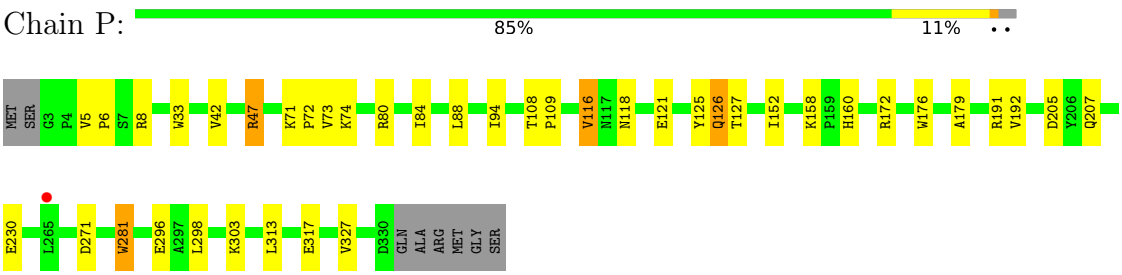
• Molecule 2: Casein kinase II subunit alpha

Chain M:



• Molecule 2: Casein kinase II subunit alpha

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	283.92Å 115.71Å 208.22Å 90.00° 119.22° 90.00°	Depositor
Resolution (Å)	181.72 – 3.50 48.31 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (181.72-3.50) 99.6 (48.31-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 3.48Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.229 , 0.259 0.228 , 0.258	Depositor DCC
R_{free} test set	3736 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	76.6	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 45.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	35073	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.83% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.62	0/1693	0.64	0/2296
1	B	0.62	1/1642 (0.1%)	0.64	0/2224
1	C	0.62	0/1668	0.62	0/2259
1	D	0.63	0/1650	0.62	0/2236
1	I	0.59	0/1650	0.61	1/2235 (0.0%)
1	J	0.59	1/1633 (0.1%)	0.61	0/2212
1	N	0.60	0/1659	0.62	0/2247
1	O	0.58	1/1667 (0.1%)	0.67	4/2259 (0.2%)
2	E	0.59	5/2851 (0.2%)	0.63	3/3856 (0.1%)
2	F	0.56	3/2841 (0.1%)	0.74	10/3842 (0.3%)
2	G	0.58	1/2851 (0.0%)	0.64	4/3856 (0.1%)
2	H	0.57	3/2845 (0.1%)	0.62	2/3848 (0.1%)
2	K	0.57	3/2845 (0.1%)	0.66	4/3848 (0.1%)
2	L	0.56	1/2845 (0.0%)	0.57	0/3848
2	M	0.57	5/2865 (0.2%)	0.58	0/3875
2	P	0.57	3/2845 (0.1%)	0.60	2/3848 (0.1%)
All	All	0.58	27/36050 (0.1%)	0.63	30/48789 (0.1%)

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
2	M	0	1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	9	TRP	CD2-CE2	6.28	1.48	1.41
2	P	176	TRP	CD2-CE2	6.21	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	281	TRP	CD2-CE2	5.88	1.48	1.41
2	E	281	TRP	CD2-CE2	5.60	1.48	1.41
1	J	9	TRP	CD2-CE2	5.55	1.48	1.41
2	L	216	TRP	CD2-CE2	5.55	1.48	1.41
2	H	216	TRP	CD2-CE2	5.54	1.48	1.41
2	E	24	TRP	CD2-CE2	5.53	1.48	1.41
2	F	216	TRP	CD2-CE2	5.50	1.48	1.41
2	K	281	TRP	CD2-CE2	5.49	1.48	1.41
2	F	24	TRP	CD2-CE2	5.46	1.47	1.41
2	P	281	TRP	CD2-CE2	5.36	1.47	1.41
2	P	33	TRP	CD2-CE2	5.32	1.47	1.41
2	H	24	TRP	CD2-CE2	5.32	1.47	1.41
2	H	33	TRP	CD2-CE2	5.28	1.47	1.41
2	K	33	TRP	CD2-CE2	5.26	1.47	1.41
2	M	24	TRP	CD2-CE2	5.26	1.47	1.41
2	E	33	TRP	CD2-CE2	5.24	1.47	1.41
2	M	33	TRP	CD2-CE2	5.22	1.47	1.41
2	M	216	TRP	CD2-CE2	5.19	1.47	1.41
2	M	176	TRP	CD2-CE2	5.11	1.47	1.41
2	K	24	TRP	CD2-CE2	5.07	1.47	1.41
2	M	281	TRP	CD2-CE2	5.07	1.47	1.41
2	F	281	TRP	CD2-CE2	5.06	1.47	1.41
2	E	176	TRP	CD2-CE2	5.01	1.47	1.41
2	E	216	TRP	CD2-CE2	5.01	1.47	1.41
1	B	9	TRP	CD2-CE2	5.00	1.47	1.41

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	120	ASP	N-CA-CB	-11.83	89.30	110.60
2	F	194	SER	N-CA-CB	-11.00	94.00	110.50
2	F	194	SER	CB-CA-C	10.41	129.88	110.10
2	G	192	VAL	N-CA-C	8.99	135.26	111.00
2	K	193	ALA	CB-CA-C	8.92	123.49	110.10
2	F	192	VAL	N-CA-C	8.77	134.67	111.00
2	K	192	VAL	CB-CA-C	-8.54	95.16	111.40
2	E	3	GLY	N-CA-C	8.28	133.79	113.10
2	F	193	ALA	N-CA-C	-8.24	88.75	111.00
2	K	192	VAL	N-CA-C	8.12	132.92	111.00
2	E	2	SER	CB-CA-C	8.02	125.33	110.10
2	H	192	VAL	N-CA-C	7.58	131.46	111.00
2	E	2	SER	N-CA-C	-7.47	90.82	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	202	GLN	CB-CA-C	-7.43	95.54	110.40
2	F	195	ARG	N-CA-C	6.90	129.63	111.00
1	O	199	LEU	N-CA-C	-6.89	92.40	111.00
2	F	195	ARG	N-CA-CB	-6.85	98.28	110.60
1	O	47	ARG	NE-CZ-NH2	6.81	123.70	120.30
2	K	193	ALA	N-CA-C	-6.34	93.88	111.00
2	H	193	ALA	N-CA-CB	-6.33	101.24	110.10
2	P	127	THR	CB-CA-C	-6.13	95.04	111.60
2	G	269	PHE	CB-CA-C	-6.09	98.22	110.40
2	G	193	ALA	N-CA-CB	-5.69	102.13	110.10
2	F	193	ALA	N-CA-CB	5.68	118.06	110.10
1	O	205	SER	CB-CA-C	-5.48	99.68	110.10
2	F	121	GLU	N-CA-CB	-5.46	100.76	110.60
1	I	205	SER	CB-CA-C	-5.40	99.84	110.10
2	P	127	THR	N-CA-C	5.23	125.11	111.00
2	F	192	VAL	CB-CA-C	-5.14	101.64	111.40
2	G	73	VAL	N-CA-C	-5.06	97.34	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	330	ASP	Peptide

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	1643	0	1556	32	0
1	B	1593	0	1519	29	0
1	C	1619	0	1535	50	0
1	D	1601	0	1524	44	0
1	I	1601	0	1523	45	0
1	J	1584	0	1513	39	0
1	N	1610	0	1529	43	0
1	O	1618	0	1534	51	0
2	E	2777	0	2719	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	2767	0	2712	23	0
2	G	2777	0	2719	34	0
2	H	2771	0	2714	21	0
2	K	2771	0	2714	25	0
2	L	2771	0	2714	36	0
2	M	2791	0	2732	30	0
2	P	2771	0	2714	21	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
All	All	35073	0	33971	453	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 7.

All (453) 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:B:193:HIS:CD2	1:B:195:MET:HB3	1.61	1.34
1:C:193:HIS:CD2	1:C:195:MET:HB3	1.61	1.33
1:I:193:HIS:HD2	1:I:195:MET:HB3	1.06	1.17
1:D:193:HIS:HD2	1:D:195:MET:HB3	1.12	1.11
1:O:193:HIS:ND1	1:O:194:PRO:HD2	1.63	1.11
1:I:193:HIS:CD2	1:I:195:MET:HB3	1.85	1.11
1:O:197:TYR:HA	1:O:200:GLN:HB2	1.35	1.09
1:C:169:MET:HE1	2:K:43:ARG:HA	1.27	1.09
2:K:194:SER:O	2:K:198:LYS:HG3	1.54	1.07
1:B:193:HIS:CD2	1:B:195:MET:CB	2.38	1.07
1:B:193:HIS:HD2	1:B:195:MET:HB3	0.89	1.05
1:O:193:HIS:CG	1:O:194:PRO:HD2	1.92	1.05
1:C:193:HIS:CD2	1:C:195:MET:CB	2.40	1.03
1:I:196:ALA:HB2	2:L:42:VAL:HA	1.34	1.03
1:C:193:HIS:HD2	1:C:195:MET:HB3	0.88	1.03
2:G:178:LEU:HD13	2:G:192:VAL:O	1.58	1.03
1:D:193:HIS:CD2	1:D:195:MET:HB3	1.96	1.00
1:O:197:TYR:CA	1:O:200:GLN:HB2	1.95	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:193:HIS:CD2	1:I:195:MET:CB	2.48	0.97
1:N:175:ARG:NH2	1:O:197:TYR:CE1	2.33	0.96
2:H:178:LEU:HD13	2:H:192:VAL:O	1.66	0.95
1:J:7:VAL:HG22	1:J:7:VAL:O	1.67	0.91
1:C:197:TYR:HE1	1:D:175:ARG:HH21	1.08	0.91
1:N:141:MET:CE	1:O:197:TYR:CD1	2.54	0.89
1:I:196:ALA:HB1	2:L:42:VAL:O	1.72	0.89
1:D:193:HIS:HD2	1:D:195:MET:CB	1.86	0.88
1:C:141:MET:CE	1:D:197:TYR:CE1	2.57	0.87
1:D:34:PHE:CZ	2:H:50:TYR:HE2	1.93	0.87
1:D:193:HIS:CD2	1:D:195:MET:CB	2.59	0.86
1:N:141:MET:HE1	1:O:197:TYR:CD1	2.11	0.86
1:O:193:HIS:CE1	1:O:194:PRO:HD2	2.10	0.85
1:O:196:ALA:CB	2:P:42:VAL:O	2.24	0.85
1:C:141:MET:HE1	1:D:197:TYR:CE1	2.12	0.84
1:N:91:ASN:HD21	2:P:47:ARG:NH1	1.73	0.84
1:B:193:HIS:HD2	1:B:195:MET:CB	1.81	0.84
1:N:193:HIS:HD2	1:N:195:MET:HB3	1.44	0.83
1:J:7:VAL:O	1:J:7:VAL:CG2	2.29	0.80
1:B:196:ALA:HB2	2:F:42:VAL:HA	1.65	0.78
1:C:197:TYR:HE1	1:D:175:ARG:NH2	1.81	0.78
1:C:193:HIS:CE1	2:H:57:ILE:HG21	2.19	0.78
2:G:303:LYS:HB3	2:G:313:LEU:HD13	1.65	0.77
2:L:103:ASP:OD1	2:L:105:VAL:HG22	1.84	0.77
1:C:193:HIS:HD2	1:C:195:MET:CB	1.81	0.77
1:N:175:ARG:NH2	1:O:197:TYR:HE1	1.78	0.77
1:I:193:HIS:HB2	2:L:40:GLN:HB3	1.66	0.77
1:I:197:TYR:CE1	1:J:141:MET:CE	2.68	0.76
1:O:193:HIS:CG	1:O:194:PRO:CD	2.67	0.76
1:O:196:ALA:HB2	2:P:42:VAL:O	1.86	0.76
2:K:269:PHE:HA	2:K:272:ILE:HD13	1.68	0.76
2:P:73:VAL:HG12	2:P:74:LYS:H	1.52	0.75
1:C:141:MET:HE3	1:D:197:TYR:CE1	2.22	0.74
1:O:196:ALA:HB1	2:P:42:VAL:O	1.87	0.74
1:D:193:HIS:O	1:D:196:ALA:HB3	1.88	0.73
1:A:193:HIS:HD2	1:A:195:MET:HB3	1.54	0.73
2:L:154:HIS:CE1	2:L:156:ASP:O	2.42	0.73
1:J:193:HIS:HD2	1:J:195:MET:HB3	1.53	0.72
1:N:141:MET:HE2	1:O:197:TYR:CD1	2.25	0.72
1:C:141:MET:HE1	1:D:197:TYR:CZ	2.25	0.72
1:I:197:TYR:CE1	1:J:141:MET:HE1	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:197:TYR:O	1:O:201:LEU:N	2.23	0.71
1:C:193:HIS:O	1:C:196:ALA:HB3	1.91	0.71
1:A:141:MET:CE	1:B:197:TYR:CD1	2.73	0.70
2:K:165:ASP:HB3	2:K:170:LYS:HB3	1.74	0.70
1:I:193:HIS:O	1:I:195:MET:N	2.25	0.69
1:I:196:ALA:HB2	2:L:42:VAL:CA	2.19	0.69
1:I:199:LEU:HD12	2:L:42:VAL:CG1	2.22	0.69
2:M:133:ILE:O	2:M:137:MET:HB2	1.92	0.69
1:D:34:PHE:CZ	2:H:50:TYR:CE2	2.79	0.68
1:J:193:HIS:HD2	1:J:195:MET:CB	2.05	0.68
2:L:103:ASP:OD2	2:L:105:VAL:HG23	1.94	0.68
1:I:197:TYR:CE1	1:J:141:MET:HE3	2.29	0.68
2:E:80:ARG:HD3	2:E:179:ALA:O	1.93	0.67
1:I:175:ARG:NH2	1:J:197:TYR:CE1	2.63	0.67
1:I:196:ALA:CB	2:L:42:VAL:O	2.43	0.67
2:L:103:ASP:OD2	2:L:105:VAL:CG2	2.42	0.67
1:I:175:ARG:NH2	1:J:197:TYR:HE1	1.93	0.67
1:A:193:HIS:CG	1:A:194:PRO:HD2	2.30	0.67
2:H:178:LEU:CD1	2:H:192:VAL:O	2.42	0.67
1:A:141:MET:HE1	1:B:197:TYR:CD1	2.30	0.67
1:N:178:ARG:CD	1:O:201:LEU:HD11	2.25	0.67
2:E:49:LYS:H	2:E:49:LYS:HD2	1.60	0.66
1:N:178:ARG:HD2	1:O:201:LEU:HD11	1.77	0.66
2:G:269:PHE:HA	2:G:272:ILE:HG12	1.76	0.66
1:B:193:HIS:O	1:B:196:ALA:N	2.28	0.66
2:G:42:VAL:HA	1:N:196:ALA:HB2	1.77	0.66
2:G:178:LEU:CD1	2:G:192:VAL:O	2.40	0.66
1:O:197:TYR:HA	1:O:200:GLN:CB	2.22	0.66
1:D:193:HIS:CD2	1:D:195:MET:H	2.14	0.65
1:N:141:MET:CE	1:O:197:TYR:HD1	2.09	0.65
1:C:43:VAL:HG12	1:C:78:MET:HG2	1.79	0.65
1:A:196:ALA:HB2	2:E:42:VAL:HA	1.78	0.65
1:I:193:HIS:ND1	1:I:194:PRO:HD2	2.12	0.64
1:I:193:HIS:CD2	1:I:195:MET:HB2	2.32	0.64
1:C:196:ALA:HB2	2:H:42:VAL:HA	1.79	0.63
1:J:196:ALA:HB2	2:M:42:VAL:HA	1.78	0.63
1:A:193:HIS:O	1:A:196:ALA:HB3	1.99	0.63
2:F:165:ASP:HB3	2:F:170:LYS:HB3	1.80	0.63
1:C:193:HIS:O	1:C:196:ALA:N	2.26	0.63
1:J:91:ASN:H	2:L:47:ARG:HH12	1.46	0.63
2:E:120:ASP:HB2	2:E:123:GLN:HE22	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:281:TRP:HB3	2:M:298:LEU:HD22	1.80	0.62
1:O:196:ALA:O	1:O:200:GLN:CG	2.47	0.62
2:G:84:ILE:HG23	2:G:152:ILE:HD13	1.80	0.62
1:J:193:HIS:CG	1:J:194:PRO:HD2	2.34	0.62
2:M:73:VAL:HG12	2:M:74:LYS:H	1.65	0.62
1:C:45:HIS:HB3	1:C:48:GLN:HG3	1.81	0.62
2:K:71:LYS:HB3	2:K:72:PRO:HD2	1.83	0.61
1:B:196:ALA:HB1	2:F:42:VAL:O	2.01	0.61
1:D:195:MET:HE1	1:D:199:LEU:HD21	1.80	0.61
1:I:193:HIS:C	1:I:195:MET:H	2.03	0.61
1:B:193:HIS:O	1:B:196:ALA:HB3	1.99	0.61
1:D:34:PHE:CE2	2:H:50:TYR:HE2	2.18	0.61
1:D:196:ALA:HB2	2:K:42:VAL:HA	1.82	0.61
1:B:202:GLN:O	1:B:204:ALA:N	2.33	0.61
1:J:202:GLN:O	1:J:204:ALA:N	2.34	0.61
1:N:195:MET:HE1	1:N:199:LEU:HD21	1.81	0.61
2:M:71:LYS:HB3	2:M:72:PRO:HD2	1.83	0.60
1:A:141:MET:HE2	1:B:197:TYR:CD1	2.36	0.60
2:K:269:PHE:O	2:K:273:LEU:HB2	2.00	0.60
1:O:196:ALA:O	1:O:200:GLN:HG3	2.02	0.60
1:D:202:GLN:O	1:D:204:ALA:N	2.35	0.60
1:J:193:HIS:ND1	1:J:194:PRO:HD2	2.17	0.59
1:N:202:GLN:O	1:N:204:ALA:N	2.35	0.59
2:F:281:TRP:HB3	2:F:298:LEU:HD22	1.85	0.59
1:B:193:HIS:CE1	2:F:57:ILE:HG21	2.38	0.58
1:N:91:ASN:ND2	2:P:47:ARG:NH1	2.50	0.58
2:M:222:LEU:O	2:M:226:ILE:HG12	2.04	0.58
1:C:202:GLN:O	1:C:204:ALA:N	2.37	0.58
1:I:193:HIS:NE2	1:I:195:MET:HB2	2.18	0.58
1:O:197:TYR:C	1:O:200:GLN:HB2	2.24	0.58
1:D:34:PHE:CE2	2:H:50:TYR:CE2	2.92	0.58
2:F:28:SER:HB2	2:L:287:SER:HB2	1.85	0.57
2:M:80:ARG:HD3	2:M:179:ALA:O	2.04	0.57
1:O:198:GLN:C	1:O:200:GLN:N	2.51	0.57
1:C:169:MET:HE2	2:K:44:LYS:H	1.70	0.57
2:G:102:LYS:HD3	2:G:107:ARG:HG3	1.85	0.57
1:I:204:ALA:O	1:I:207:PHE:HB2	2.04	0.57
1:N:178:ARG:HD2	1:O:201:LEU:CD1	2.35	0.57
1:A:91:ASN:OD1	2:F:47:ARG:NH1	2.37	0.56
1:C:193:HIS:O	1:C:196:ALA:CB	2.51	0.56
1:O:51:ASP:HB2	1:O:56:LEU:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:MET:HE1	1:C:199:LEU:HD21	1.87	0.56
1:I:196:ALA:CB	2:L:42:VAL:HA	2.23	0.56
1:C:165:HIS:CE1	1:D:185:PRO:HB3	2.41	0.56
1:C:196:ALA:HB1	2:H:42:VAL:O	2.06	0.56
2:L:103:ASP:CG	2:L:105:VAL:CG2	2.74	0.56
1:A:202:GLN:O	1:A:204:ALA:N	2.39	0.56
1:I:195:MET:HE1	1:I:199:LEU:HD21	1.86	0.56
1:C:204:ALA:O	1:C:207:PHE:HB2	2.06	0.56
1:A:195:MET:HE3	1:A:199:LEU:HD11	1.88	0.55
2:F:192:VAL:HG23	2:F:202:LEU:HD13	1.88	0.55
1:J:193:HIS:O	1:J:195:MET:N	2.39	0.55
1:D:195:MET:CE	1:D:199:LEU:HD21	2.36	0.55
2:G:50:TYR:CE2	1:O:34:PHE:HZ	2.24	0.55
2:H:158:LYS:HD2	2:H:160:HIS:HB2	1.88	0.55
1:C:169:MET:HE3	1:C:169:MET:HA	1.88	0.55
1:C:195:MET:CE	1:C:199:LEU:HD21	2.37	0.55
1:D:193:HIS:CG	1:D:194:PRO:HD2	2.41	0.55
1:N:193:HIS:CD2	1:N:195:MET:HB3	2.34	0.55
1:B:193:HIS:CD2	1:B:195:MET:HB2	2.37	0.55
2:G:281:TRP:HB3	2:G:298:LEU:HD22	1.88	0.55
1:J:193:HIS:CD2	1:J:195:MET:CB	2.89	0.55
1:N:178:ARG:CD	1:O:201:LEU:CD1	2.85	0.55
1:A:196:ALA:HB1	2:E:42:VAL:O	2.07	0.55
1:N:193:HIS:HD2	1:N:195:MET:CB	2.16	0.55
1:N:202:GLN:C	1:N:204:ALA:H	2.11	0.55
1:N:204:ALA:HA	1:O:173:GLU:HA	1.89	0.55
2:E:195:ARG:HH22	1:O:70:ASP:CG	2.09	0.55
1:I:202:GLN:C	1:I:204:ALA:N	2.60	0.55
2:M:116:VAL:HG21	2:M:172:ARG:HG3	1.89	0.55
1:N:204:ALA:O	1:N:207:PHE:HB2	2.06	0.55
1:N:202:GLN:C	1:N:204:ALA:N	2.60	0.54
1:A:204:ALA:O	1:A:207:PHE:HB2	2.08	0.54
1:D:202:GLN:C	1:D:204:ALA:N	2.60	0.54
2:G:120:ASP:HB2	2:G:123:GLN:HE22	1.72	0.54
1:D:204:ALA:O	1:D:207:PHE:HB2	2.07	0.54
1:I:202:GLN:C	1:I:204:ALA:H	2.11	0.54
1:N:193:HIS:CG	1:N:194:PRO:HD2	2.43	0.54
2:G:40:GLN:HG2	1:N:191:LYS:HB3	1.89	0.54
1:I:202:GLN:O	1:I:204:ALA:N	2.39	0.54
2:P:313:LEU:HD22	2:P:317:GLU:HB3	1.89	0.54
1:D:202:GLN:C	1:D:204:ALA:H	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:134:ARG:HG2	2:F:323:TYR:CZ	2.43	0.54
1:J:90:THR:HA	2:L:47:ARG:HH22	1.72	0.54
2:F:118:ASN:HB3	2:F:163:MET:SD	2.48	0.54
2:F:222:LEU:O	2:F:226:ILE:HG12	2.08	0.54
1:A:202:GLN:C	1:A:204:ALA:N	2.61	0.54
1:D:195:MET:O	1:D:199:LEU:HG	2.08	0.54
2:G:222:LEU:O	2:G:226:ILE:HG12	2.08	0.54
1:I:43:VAL:HG21	1:I:79:LEU:HD13	1.90	0.54
1:J:202:GLN:C	1:J:204:ALA:H	2.10	0.54
1:B:204:ALA:O	1:B:207:PHE:HB2	2.08	0.54
1:B:206:ASN:O	1:B:207:PHE:C	2.47	0.53
1:C:206:ASN:O	1:C:207:PHE:C	2.47	0.53
1:J:202:GLN:C	1:J:204:ALA:N	2.60	0.53
1:J:204:ALA:O	1:J:207:PHE:HB2	2.09	0.53
2:P:71:LYS:HB3	2:P:72:PRO:HD2	1.90	0.53
1:J:196:ALA:HB1	2:M:42:VAL:O	2.08	0.53
1:J:202:GLN:O	1:J:205:SER:N	2.42	0.53
1:N:195:MET:O	1:N:199:LEU:HG	2.08	0.53
2:E:135:PHE:HA	2:E:327:VAL:HG21	1.89	0.53
1:N:141:MET:HE2	1:O:197:TYR:HD1	1.69	0.53
1:O:196:ALA:O	1:O:200:GLN:NE2	2.42	0.53
1:C:169:MET:CE	2:K:43:ARG:HA	2.20	0.53
1:B:202:GLN:O	1:B:205:SER:N	2.42	0.53
1:J:195:MET:CE	1:J:199:LEU:HD21	2.39	0.53
1:D:202:GLN:O	1:D:205:SER:N	2.42	0.53
1:N:202:GLN:O	1:N:205:SER:N	2.42	0.53
1:A:206:ASN:O	1:A:207:PHE:C	2.47	0.53
2:K:194:SER:O	2:K:198:LYS:CG	2.44	0.53
1:O:206:ASN:O	1:O:207:PHE:C	2.47	0.53
2:L:280:ARG:HH11	2:L:280:ARG:CG	2.22	0.53
1:C:202:GLN:C	1:C:204:ALA:N	2.60	0.52
1:J:206:ASN:O	1:J:207:PHE:C	2.48	0.52
1:B:202:GLN:C	1:B:204:ALA:H	2.10	0.52
1:C:141:MET:HE3	1:D:197:TYR:HE1	1.74	0.52
1:C:202:GLN:C	1:C:204:ALA:H	2.11	0.52
1:N:195:MET:CE	1:N:199:LEU:HD21	2.39	0.52
1:N:206:ASN:O	1:N:207:PHE:C	2.46	0.52
2:M:255:TYR:HA	2:M:258:ILE:HG12	1.92	0.52
1:O:204:ALA:O	1:O:207:PHE:HB2	2.09	0.52
1:D:206:ASN:O	1:D:207:PHE:C	2.47	0.52
1:A:193:HIS:HD2	1:A:195:MET:CB	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:GLN:C	1:B:204:ALA:N	2.59	0.51
1:A:65:ASN:HB3	1:A:68:GLN:HB2	1.92	0.51
2:H:231:PRO:HD2	2:H:234:HIS:ND1	2.25	0.51
1:O:65:ASN:HB2	1:O:68:GLN:HB2	1.93	0.51
1:B:193:HIS:O	1:B:196:ALA:CB	2.58	0.51
1:A:202:GLN:C	1:A:204:ALA:H	2.12	0.51
2:E:134:ARG:HG2	2:E:323:TYR:CZ	2.45	0.51
1:J:193:HIS:C	1:J:195:MET:H	2.13	0.51
1:C:52:MET:HE1	1:C:73:GLU:HA	1.93	0.51
1:C:202:GLN:O	1:C:205:SER:N	2.44	0.51
2:E:328:VAL:HG13	2:E:329:LYS:HG2	1.92	0.51
2:P:88:LEU:HB3	2:P:94:ILE:HG21	1.93	0.51
1:I:195:MET:O	1:I:199:LEU:HG	2.11	0.51
1:J:67:ASN:OD1	1:J:67:ASN:O	2.28	0.51
1:N:200:GLN:OE1	1:O:175:ARG:HD3	2.11	0.51
1:D:37:THR:HG21	2:H:73:VAL:O	2.10	0.51
1:I:199:LEU:CD1	2:L:42:VAL:CG1	2.88	0.51
1:N:28:ASP:OD1	1:N:28:ASP:N	2.44	0.51
1:C:178:ARG:HH11	1:D:201:LEU:CD1	2.24	0.50
2:E:165:ASP:HB3	2:E:170:LYS:HB3	1.93	0.50
1:I:195:MET:CE	1:I:199:LEU:HD21	2.41	0.50
2:P:281:TRP:HB3	2:P:298:LEU:HD22	1.94	0.50
1:N:195:MET:HE3	1:N:199:LEU:HD11	1.94	0.50
1:A:165:HIS:O	1:A:169:MET:HG2	2.12	0.50
1:B:191:LYS:HB2	2:F:40:GLN:HG2	1.93	0.50
2:E:281:TRP:HB3	2:E:298:LEU:HD22	1.94	0.50
1:C:166:MET:HG2	1:D:187:LEU:HD21	1.94	0.50
2:H:119:THR:HB	2:H:124:LEU:HD23	1.93	0.50
1:I:195:MET:HE3	1:I:199:LEU:HD11	1.94	0.50
1:O:196:ALA:O	1:O:200:GLN:CD	2.49	0.50
1:C:193:HIS:CD2	1:C:195:MET:HB2	2.41	0.49
2:H:158:LYS:HE2	2:H:194:SER:OG	2.12	0.49
1:C:185:PRO:HB3	1:D:165:HIS:CE1	2.48	0.49
1:C:195:MET:O	1:C:199:LEU:HG	2.11	0.49
1:I:206:ASN:O	1:I:207:PHE:C	2.49	0.49
1:A:202:GLN:O	1:A:205:SER:N	2.46	0.49
2:M:240:ASP:O	2:M:244:ARG:HG2	2.13	0.49
1:I:193:HIS:C	1:I:195:MET:N	2.64	0.48
1:O:198:GLN:O	1:O:202:GLN:HG3	2.12	0.48
2:G:5:VAL:HB	2:G:261:TYR:HA	1.95	0.48
1:A:195:MET:CE	1:A:199:LEU:HD21	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:71:LYS:O	2:K:73:VAL:HG23	2.13	0.48
2:M:322:PRO:HA	2:M:325:TYR:CD2	2.48	0.48
2:G:134:ARG:HG2	2:G:323:TYR:CZ	2.48	0.48
2:P:116:VAL:HG11	2:P:172:ARG:HG3	1.94	0.48
2:G:313:LEU:HD23	2:G:318:ALA:HA	1.96	0.48
1:J:195:MET:O	1:J:199:LEU:HG	2.13	0.48
2:F:80:ARG:HH22	2:F:155:ARG:NH2	2.12	0.48
1:I:202:GLN:O	1:I:205:SER:N	2.47	0.48
1:D:111:ARG:NH1	1:D:114:CYS:SG	2.86	0.48
1:D:193:HIS:CD2	1:D:195:MET:HB2	2.45	0.48
2:K:192:VAL:C	2:K:193:ALA:O	2.51	0.48
1:I:189:GLY:HA3	2:L:103:ASP:CG	2.33	0.48
1:I:199:LEU:HD12	2:L:42:VAL:HG13	1.94	0.47
2:K:195:ARG:O	2:K:241:GLN:HG2	2.14	0.47
2:L:303:LYS:HB3	2:L:313:LEU:HG	1.96	0.47
2:M:223:ALA:HB2	2:M:301:LEU:HD11	1.96	0.47
1:N:165:HIS:CE1	1:O:185:PRO:HB3	2.49	0.47
1:O:197:TYR:C	1:O:200:GLN:H	2.18	0.47
1:J:195:MET:HE1	1:J:199:LEU:HD21	1.96	0.47
1:N:43:VAL:HG12	1:N:78:MET:HG2	1.95	0.47
1:I:111:ARG:NH1	1:I:114:CYS:SG	2.87	0.47
2:P:84:ILE:HG23	2:P:152:ILE:HD13	1.96	0.47
2:E:116:VAL:HG11	2:E:172:ARG:HG3	1.97	0.47
1:A:111:ARG:NH1	1:A:114:CYS:SG	2.87	0.47
1:A:195:MET:O	1:A:199:LEU:HG	2.15	0.47
1:B:193:HIS:C	1:B:195:MET:N	2.68	0.47
2:G:226:ILE:O	2:G:289:ASN:HB2	2.14	0.47
1:I:165:HIS:CE1	1:J:185:PRO:HB3	2.50	0.47
1:C:141:MET:CE	1:D:197:TYR:CZ	2.91	0.47
2:E:222:LEU:O	2:E:226:ILE:HG12	2.15	0.47
2:L:154:HIS:ND1	2:L:156:ASP:O	2.46	0.47
1:O:193:HIS:CD2	1:O:194:PRO:HD2	2.45	0.47
2:P:80:ARG:HD3	2:P:179:ALA:O	2.15	0.47
2:G:73:VAL:HG12	2:G:74:LYS:H	1.80	0.47
2:M:33:TRP:CE3	2:M:102:LYS:HB2	2.49	0.47
2:M:158:LYS:HG3	2:M:160:HIS:H	1.80	0.47
1:C:165:HIS:O	1:C:169:MET:HG2	2.14	0.46
1:N:205:SER:O	1:N:206:ASN:C	2.53	0.46
1:A:43:VAL:HG12	1:A:78:MET:HG2	1.96	0.46
2:H:281:TRP:HB3	2:H:298:LEU:HD22	1.97	0.46
1:N:193:HIS:CD2	1:N:195:MET:CB	2.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:193:HIS:CG	1:O:194:PRO:N	2.83	0.46
1:C:88:ILE:HA	1:C:93:GLY:HA3	1.97	0.46
1:I:189:GLY:HA3	2:L:103:ASP:OD2	2.15	0.46
1:I:186:ARG:HH21	1:I:191:LYS:HE3	1.80	0.46
2:G:50:TYR:CE2	1:O:34:PHE:CZ	3.04	0.46
1:D:66:PRO:O	1:D:70:ASP:HB2	2.16	0.46
1:D:193:HIS:O	1:D:196:ALA:CB	2.60	0.45
2:K:258:ILE:HG21	2:K:265:LEU:HD21	1.97	0.45
2:M:325:TYR:HA	2:M:328:VAL:HG12	1.97	0.45
1:A:165:HIS:CE1	1:B:185:PRO:HB3	2.51	0.45
2:M:165:ASP:HB3	2:M:170:LYS:HB3	1.96	0.45
1:N:88:ILE:O	1:N:94:ILE:HG13	2.16	0.45
2:P:126:GLN:H	2:P:126:GLN:HE21	1.64	0.45
2:G:328:VAL:O	2:G:328:VAL:HG13	2.16	0.45
2:L:281:TRP:HB3	2:L:298:LEU:HD22	1.97	0.45
1:C:117:GLN:HG2	1:C:139:LYS:HB2	1.98	0.45
2:G:66:VAL:HG23	2:G:115:HIS:HA	1.98	0.45
2:K:80:ARG:HD3	2:K:179:ALA:O	2.17	0.45
1:O:198:GLN:C	1:O:200:GLN:H	2.15	0.45
2:G:10:ARG:HH21	2:G:314:THR:HG23	1.80	0.45
2:H:80:ARG:HD3	2:H:179:ALA:O	2.16	0.45
2:P:121:GLU:O	2:P:125:TYR:HB2	2.16	0.45
2:E:286:HIS:ND1	2:E:288:GLU:HG2	2.31	0.45
2:L:322:PRO:HA	2:L:325:TYR:CD2	2.51	0.45
1:N:141:MET:CE	1:O:197:TYR:CE1	2.98	0.45
2:G:183:HIS:HB2	2:G:186:GLN:HE21	1.80	0.45
1:J:193:HIS:CD2	1:J:195:MET:HB2	2.52	0.45
2:L:103:ASP:CG	2:L:105:VAL:HG22	2.33	0.45
1:D:163:PHE:HB3	1:D:164:PRO:HD3	1.98	0.45
2:F:71:LYS:HB3	2:F:72:PRO:HD2	1.98	0.45
2:H:165:ASP:HB3	2:H:170:LYS:HB3	1.98	0.45
1:N:120:LEU:HD21	1:N:167:LEU:HD13	1.99	0.45
2:M:96:THR:HB	2:M:114:GLU:HB2	1.99	0.44
2:L:103:ASP:CG	2:L:105:VAL:HG23	2.36	0.44
1:C:205:SER:O	1:C:206:ASN:C	2.56	0.44
2:F:118:ASN:CB	2:F:163:MET:SD	3.05	0.44
2:L:230:GLU:HA	2:L:231:PRO:HA	1.87	0.44
1:C:197:TYR:CE1	1:D:175:ARG:NH2	2.62	0.44
1:D:205:SER:O	1:D:206:ASN:C	2.56	0.44
2:H:27:GLU:HG2	2:H:76:LYS:HG3	1.99	0.44
2:K:136:TYR:O	2:K:140:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:162:GLY:HA2	1:J:165:HIS:HD2	1.82	0.44
1:A:112:VAL:HG11	1:B:124:LEU:HD11	1.99	0.44
2:K:222:LEU:O	2:K:226:ILE:HG12	2.18	0.44
2:K:230:GLU:HA	2:K:231:PRO:HA	1.85	0.44
2:G:254:LEU:HD21	2:G:273:LEU:HD21	2.00	0.44
2:M:53:VAL:HG22	2:M:68:LYS:HG3	1.98	0.44
1:A:141:MET:HE2	1:B:197:TYR:CE1	2.52	0.44
1:D:25:VAL:HG13	1:D:87:TYR:CD1	2.52	0.44
1:O:149:SER:HA	1:O:152:HIS:CD2	2.52	0.44
2:F:193:ALA:O	2:F:194:SER:C	2.55	0.43
2:G:8:ARG:HH21	2:G:184:PRO:HB2	1.83	0.43
2:G:266:ASP:HB3	2:G:269:PHE:HD1	1.82	0.43
2:K:239:TYR:CZ	2:K:268:ARG:HD2	2.52	0.43
1:N:175:ARG:NH2	1:O:197:TYR:CD1	2.69	0.43
1:C:149:SER:HA	1:C:152:HIS:CE1	2.53	0.43
2:F:84:ILE:HG23	2:F:152:ILE:HD13	1.99	0.43
2:F:120:ASP:C	2:F:122:LYS:N	2.71	0.43
2:G:45:LEU:HD11	2:G:55:GLU:HB2	2.01	0.43
1:I:199:LEU:HD12	2:L:42:VAL:HG12	1.99	0.43
2:L:71:LYS:HG2	2:L:72:PRO:HD2	2.00	0.43
2:L:103:ASP:OD1	2:L:104:PRO:HD2	2.19	0.43
2:L:108:THR:HA	2:L:109:PRO:HD3	1.83	0.43
1:O:165:HIS:O	1:O:169:MET:HG2	2.18	0.43
2:G:108:THR:HA	2:G:109:PRO:HD3	1.87	0.43
2:M:294:SER:H	2:M:297:ALA:HB3	1.83	0.43
2:F:303:LYS:HB3	2:F:313:LEU:HG	2.01	0.43
1:I:149:SER:HA	1:I:152:HIS:ND1	2.33	0.43
2:L:5:VAL:HB	2:L:261:TYR:HA	2.00	0.43
2:M:51:SER:HB2	2:M:68:LYS:HG2	2.00	0.43
1:O:127:ILE:HB	1:O:130:GLU:HG3	2.00	0.43
1:A:182:GLN:HE21	1:A:182:GLN:HB3	1.71	0.43
2:K:195:ARG:O	2:K:241:GLN:CD	2.56	0.43
2:M:139:GLU:HB2	2:M:171:LEU:HD13	2.01	0.43
2:P:303:LYS:HB3	2:P:313:LEU:HG	2.01	0.43
1:A:192:ILE:HG22	1:A:197:TYR:CE2	2.54	0.43
1:C:88:ILE:O	1:C:94:ILE:HG13	2.19	0.43
1:I:193:HIS:CG	1:I:194:PRO:HD2	2.54	0.43
1:J:193:HIS:C	1:J:195:MET:N	2.71	0.43
1:J:127:ILE:HA	1:J:128:PRO:HD3	1.91	0.43
1:C:135:LEU:HG	1:C:146:PRO:HG3	2.01	0.42
1:C:193:HIS:C	1:C:195:MET:N	2.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:35:ASN:HD22	2:G:37:ASP:H	1.66	0.42
1:N:91:ASN:HD21	2:P:47:ARG:CZ	2.29	0.42
1:O:175:ARG:HA	1:O:176:PRO:HD3	1.83	0.42
1:A:175:ARG:NH2	1:B:197:TYR:HE1	2.18	0.42
2:F:124:LEU:CD1	2:F:166:HIS:HD2	2.32	0.42
2:G:93:ASN:ND2	2:G:139:GLU:HB3	2.34	0.42
2:K:98:ALA:HB2	2:K:114:GLU:HG3	2.01	0.42
1:A:186:ARG:O	1:B:161:THR:HG23	2.19	0.42
2:E:108:THR:HA	2:E:109:PRO:HD3	1.93	0.42
1:J:191:LYS:HB2	2:M:40:GLN:HG2	2.01	0.42
2:G:199:GLY:HA2	2:G:216:TRP:CD1	2.54	0.42
1:B:43:VAL:HG12	1:B:78:MET:SD	2.59	0.42
2:E:230:GLU:HA	2:E:231:PRO:HA	1.90	0.42
2:M:36:GLN:HE21	2:M:104:PRO:HD2	1.85	0.42
2:E:303:LYS:HB3	2:E:313:LEU:HG	2.02	0.42
2:G:10:ARG:NH2	2:G:317:GLU:OE1	2.53	0.42
2:E:71:LYS:O	2:E:73:VAL:HG23	2.20	0.42
1:I:197:TYR:CZ	1:J:141:MET:HE1	2.55	0.42
2:L:280:ARG:HH11	2:L:280:ARG:HG3	1.83	0.42
2:L:290:GLN:HE21	2:L:290:GLN:HB2	1.57	0.42
2:M:5:VAL:HB	2:M:261:TYR:HA	2.02	0.42
2:F:327:VAL:O	2:F:328:VAL:C	2.58	0.42
2:P:5:VAL:HA	2:P:6:PRO:HD3	1.91	0.42
2:G:36:GLN:HE21	2:G:36:GLN:HB3	1.60	0.42
2:E:200:PRO:O	2:E:204:VAL:HG22	2.20	0.41
2:H:186:GLN:HG2	2:H:188:TYR:CZ	2.55	0.41
1:N:141:MET:HE2	1:O:197:TYR:CE1	2.54	0.41
2:F:106:SER:O	2:F:107:ARG:HB2	2.20	0.41
2:F:155:ARG:O	2:F:193:ALA:HB2	2.20	0.41
2:K:239:TYR:CE2	2:K:268:ARG:HD2	2.55	0.41
2:M:230:GLU:HA	2:M:231:PRO:HA	1.89	0.41
1:O:198:GLN:N	1:O:200:GLN:H	2.18	0.41
2:P:108:THR:HA	2:P:109:PRO:HD3	1.87	0.41
1:B:139:LYS:HG2	1:B:179:PRO:HD3	2.02	0.41
2:E:122:LYS:H	2:E:122:LYS:HD2	1.85	0.41
2:E:5:VAL:HB	2:E:261:TYR:HA	2.02	0.41
2:K:134:ARG:HG2	2:K:323:TYR:CZ	2.56	0.41
1:A:195:MET:HE3	1:A:199:LEU:HD21	2.01	0.41
2:E:123:GLN:HE21	2:E:123:GLN:HB2	1.71	0.41
2:E:199:GLY:HA2	2:E:216:TRP:CD1	2.55	0.41
2:H:327:VAL:O	2:H:329:LYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:101:TYR:CD1	1:I:120:LEU:HD13	2.55	0.41
2:L:122:LYS:HD2	2:L:122:LYS:H	1.85	0.41
1:D:196:ALA:CB	2:K:42:VAL:HA	2.47	0.41
2:G:325:TYR:HA	2:G:328:VAL:HG12	2.03	0.41
1:I:36:LEU:HD22	1:I:83:ILE:HG12	2.03	0.41
2:K:3:GLY:HA2	2:K:4:PRO:HD3	1.90	0.41
1:N:137:CYS:HA	1:N:138:PRO:HD3	1.86	0.41
2:M:316:ARG:O	2:M:320:GLU:HG2	2.21	0.41
2:M:321:HIS:CG	2:M:322:PRO:HD2	2.56	0.41
2:H:116:VAL:HG21	2:H:172:ARG:HG3	2.03	0.41
1:J:57:GLU:HA	1:J:58:PRO:HD3	1.90	0.41
1:J:205:SER:O	1:J:206:ASN:C	2.59	0.41
2:M:71:LYS:CB	2:M:72:PRO:HD2	2.50	0.41
2:M:134:ARG:HG2	2:M:323:TYR:CZ	2.55	0.41
2:G:255:TYR:HA	2:G:258:ILE:HG12	2.02	0.40
1:D:184:VAL:HA	1:D:185:PRO:HD3	1.88	0.40
1:J:186:ARG:HA	1:J:190:PHE:O	2.21	0.40
2:L:199:GLY:HA2	2:L:216:TRP:CD1	2.56	0.40
2:E:91:GLY:HA3	2:E:146:TYR:CE2	2.56	0.40
1:A:8:SER:HB3	1:A:11:SER:HB2	2.04	0.40
1:C:137:CYS:HA	1:C:138:PRO:HD3	1.96	0.40
1:C:175:ARG:HA	1:C:176:PRO:HD3	1.92	0.40
1:J:138:PRO:HB3	1:J:168:PHE:CZ	2.56	0.40
2:P:73:VAL:HG12	2:P:74:LYS:N	2.30	0.40
2:P:158:LYS:HD2	2:P:160:HIS:HB2	2.04	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	199/215 (93%)	194 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	191/215 (89%)	184 (96%)	7 (4%)	0	100	100
1	C	194/215 (90%)	187 (96%)	7 (4%)	0	100	100
1	D	192/215 (89%)	184 (96%)	8 (4%)	0	100	100
1	I	192/215 (89%)	183 (95%)	8 (4%)	1 (0%)	29	68
1	J	190/215 (88%)	184 (97%)	5 (3%)	1 (0%)	29	68
1	N	193/215 (90%)	188 (97%)	5 (3%)	0	100	100
1	O	194/215 (90%)	191 (98%)	3 (2%)	0	100	100
2	E	327/336 (97%)	313 (96%)	13 (4%)	1 (0%)	41	75
2	F	325/336 (97%)	299 (92%)	24 (7%)	2 (1%)	25	64
2	G	327/336 (97%)	303 (93%)	23 (7%)	1 (0%)	41	75
2	H	326/336 (97%)	304 (93%)	21 (6%)	1 (0%)	41	75
2	K	326/336 (97%)	311 (95%)	14 (4%)	1 (0%)	41	75
2	L	326/336 (97%)	311 (95%)	15 (5%)	0	100	100
2	M	329/336 (98%)	309 (94%)	19 (6%)	1 (0%)	41	75
2	P	326/336 (97%)	307 (94%)	19 (6%)	0	100	100
All	All	4157/4408 (94%)	3952 (95%)	196 (5%)	9 (0%)	47	81

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	194	PRO
1	J	194	PRO
2	F	50	TYR
2	H	328	VAL
2	K	328	VAL
2	M	330	ASP
2	G	328	VAL
2	F	328	VAL
2	E	328	VAL

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	177/191 (93%)	170 (96%)	7 (4%)	31	64
1	B	171/191 (90%)	167 (98%)	4 (2%)	50	77
1	C	174/191 (91%)	164 (94%)	10 (6%)	20	53
1	D	172/191 (90%)	166 (96%)	6 (4%)	36	67
1	I	172/191 (90%)	163 (95%)	9 (5%)	23	56
1	J	170/191 (89%)	167 (98%)	3 (2%)	59	81
1	N	173/191 (91%)	162 (94%)	11 (6%)	17	50
1	O	174/191 (91%)	170 (98%)	4 (2%)	50	77
2	E	303/308 (98%)	290 (96%)	13 (4%)	29	62
2	F	302/308 (98%)	295 (98%)	7 (2%)	50	77
2	G	303/308 (98%)	290 (96%)	13 (4%)	29	62
2	H	302/308 (98%)	287 (95%)	15 (5%)	24	58
2	K	302/308 (98%)	285 (94%)	17 (6%)	21	54
2	L	302/308 (98%)	291 (96%)	11 (4%)	35	66
2	M	304/308 (99%)	288 (95%)	16 (5%)	22	55
2	P	302/308 (98%)	289 (96%)	13 (4%)	29	62
All	All	3803/3992 (95%)	3644 (96%)	159 (4%)	30	63

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LYS
1	A	47	ARG
1	A	57	GLU
1	A	73	GLU
1	A	120	LEU
1	A	182	GLN
1	A	207	PHE
1	B	166	MET
1	B	175	ARG
1	B	178	ARG
1	B	207	PHE
1	C	17	ARG
1	C	28	ASP
1	C	33	LYS
1	C	48	GLN

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Mol	Chain	Res	Type
1	C	57	GLU
1	C	92	ARG
1	C	120	LEU
1	C	166	MET
1	C	184	VAL
1	C	207	PHE
1	D	7	VAL
1	D	17	ARG
1	D	52	MET
1	D	132	MET
1	D	182	GLN
1	D	207	PHE
2	E	40	GLN
2	E	52	GLU
2	E	76	LYS
2	E	118	ASN
2	E	121	GLU
2	E	123	GLN
2	E	236	HIS
2	E	252	GLU
2	E	269	PHE
2	E	270	ASN
2	E	279	LYS
2	E	293	VAL
2	E	330	ASP
2	F	73	VAL
2	F	105	VAL
2	F	119	THR
2	F	121	GLU
2	F	192	VAL
2	F	205	ASP
2	F	268	ARG
2	G	21	ARG
2	G	35	ASN
2	G	36	GLN
2	G	63	GLU
2	G	65	VAL
2	G	103	ASP
2	G	108	THR
2	G	121	GLU
2	G	122	LYS
2	G	123	GLN

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Mol	Chain	Res	Type
2	G	125	TYR
2	G	265	LEU
2	G	290	GLN
2	H	40	GLN
2	H	43	ARG
2	H	47	ARG
2	H	49	LYS
2	H	65	VAL
2	H	107	ARG
2	H	119	THR
2	H	127	THR
2	H	186	GLN
2	H	236	HIS
2	H	278	ARG
2	H	280	ARG
2	H	290	GLN
2	H	316	ARG
2	H	329	LYS
1	I	28	ASP
1	I	48	GLN
1	I	57	GLU
1	I	92	ARG
1	I	120	LEU
1	I	147	LYS
1	I	166	MET
1	I	184	VAL
1	I	207	PHE
1	J	7	VAL
1	J	132	MET
1	J	207	PHE
2	K	35	ASN
2	K	36	GLN
2	K	52	GLU
2	K	77	LYS
2	K	116	VAL
2	K	118	ASN
2	K	119	THR
2	K	126	GLN
2	K	127	THR
2	K	175	ASP
2	K	192	VAL
2	K	194	SER

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Mol	Chain	Res	Type
2	K	272	ILE
2	K	273	LEU
2	K	283	ARG
2	K	290	GLN
2	K	303	LYS
2	L	10	ARG
2	L	35	ASN
2	L	40	GLN
2	L	47	ARG
2	L	71	LYS
2	L	105	VAL
2	L	228	ARG
2	L	244	ARG
2	L	278	ARG
2	L	280	ARG
2	L	290	GLN
2	M	8	ARG
2	M	36	GLN
2	M	44	LYS
2	M	47	ARG
2	M	65	VAL
2	M	100	ILE
2	M	107	ARG
2	M	167	GLU
2	M	175	ASP
2	M	186	GLN
2	M	202	LEU
2	M	252	GLU
2	M	264	GLU
2	M	271	ASP
2	M	283	ARG
2	M	329	LYS
1	N	28	ASP
1	N	42	GLN
1	N	47	ARG
1	N	70	ASP
1	N	92	ARG
1	N	120	LEU
1	N	132	MET
1	N	169	MET
1	N	175	ARG
1	N	184	VAL

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Mol	Chain	Res	Type
1	N	207	PHE
1	O	7	VAL
1	O	132	MET
1	O	175	ARG
1	O	207	PHE
2	P	8	ARG
2	P	47	ARG
2	P	116	VAL
2	P	118	ASN
2	P	126	GLN
2	P	191	ARG
2	P	192	VAL
2	P	205	ASP
2	P	207	GLN
2	P	230	GLU
2	P	271	ASP
2	P	296	GLU
2	P	327	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	GLN
1	A	193	HIS
1	B	91	ASN
1	B	193	HIS
1	C	42	GLN
1	C	165	HIS
1	C	182	GLN
1	C	193	HIS
1	D	45	HIS
1	D	102	GLN
1	D	165	HIS
1	D	193	HIS
2	E	123	GLN
2	E	126	GLN
2	F	186	GLN
2	F	270	ASN
2	G	35	ASN
2	G	123	GLN
2	G	186	GLN
2	G	276	HIS

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Mol	Chain	Res	Type
2	H	18	HIS
2	H	36	GLN
2	H	186	GLN
2	H	290	GLN
1	I	48	GLN
1	I	102	GLN
1	I	165	HIS
1	I	182	GLN
1	I	193	HIS
1	J	45	HIS
1	J	165	HIS
1	J	193	HIS
2	K	35	ASN
2	K	290	GLN
2	L	35	ASN
2	L	36	GLN
2	L	123	GLN
2	L	290	GLN
2	L	310	GLN
2	M	18	HIS
2	M	36	GLN
1	N	42	GLN
1	N	91	ASN
1	N	102	GLN
1	N	165	HIS
1	N	182	GLN
1	N	193	HIS
1	O	165	HIS
1	O	193	HIS
2	P	35	ASN
2	P	40	GLN
2	P	123	GLN
2	P	126	GLN
2	P	290	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 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 (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 (i)

6.1 Protein, DNA and RNA chains (i)

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	201/215 (93%)	-0.31	0 100 100	55, 81, 125, 152	0
1	B	195/215 (90%)	-0.26	1 (0%) 91 88	57, 77, 108, 135	0
1	C	198/215 (92%)	-0.31	0 100 100	55, 78, 124, 167	0
1	D	196/215 (91%)	-0.36	0 100 100	55, 76, 109, 142	0
1	I	196/215 (91%)	-0.23	1 (0%) 91 88	62, 86, 118, 135	0
1	J	194/215 (90%)	-0.17	0 100 100	58, 93, 122, 142	0
1	N	197/215 (91%)	-0.22	0 100 100	58, 92, 121, 140	0
1	O	198/215 (92%)	-0.05	5 (2%) 57 51	72, 102, 141, 178	0
2	E	329/336 (97%)	-0.20	2 (0%) 89 86	51, 92, 124, 153	0
2	F	327/336 (97%)	-0.22	2 (0%) 89 86	60, 87, 116, 134	0
2	G	329/336 (97%)	-0.34	0 100 100	59, 81, 109, 125	0
2	H	328/336 (97%)	-0.28	0 100 100	63, 90, 116, 126	0
2	K	328/336 (97%)	-0.23	2 (0%) 89 86	59, 84, 110, 148	0
2	L	328/336 (97%)	-0.16	1 (0%) 94 91	65, 94, 123, 154	0
2	M	331/336 (98%)	-0.12	1 (0%) 94 91	66, 89, 115, 129	0
2	P	328/336 (97%)	-0.23	1 (0%) 94 91	71, 93, 119, 148	0
All	All	4203/4408 (95%)	-0.23	16 (0%) 92 90	51, 88, 120, 178	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	68	GLN	4.9
2	L	120	ASP	3.0
1	O	56	LEU	2.8
2	K	6	PRO	2.6
2	M	184	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	206	ASN	2.4
2	P	265	LEU	2.3
2	F	122	LYS	2.2
1	O	46	TYR	2.2
2	F	123	GLN	2.2
1	I	203	ALA	2.1
2	K	4	PRO	2.1
1	O	10	ILE	2.1
2	E	276	HIS	2.0
2	E	120	ASP	2.0
1	O	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	N	301	1/1	0.98	0.14	73,73,73,73	0
3	ZN	D	301	1/1	0.99	0.14	63,63,63,63	0
3	ZN	I	301	1/1	0.99	0.12	70,70,70,70	0
3	ZN	J	301	1/1	0.99	0.11	77,77,77,77	0
3	ZN	B	301	1/1	0.99	0.11	66,66,66,66	0
3	ZN	O	301	1/1	0.99	0.12	59,59,59,59	0
3	ZN	C	301	1/1	1.00	0.16	63,63,63,63	0
3	ZN	A	301	1/1	1.00	0.10	58,58,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.