Full wwPDB X-ray Structure Validation Report (i)

Nov 2, 2016 – 11:10 AM EDT

PDB ID	:	5EJG
Title	:	Crystal structure of NAD kinase P252D mutant from Listeria monocytogenes
Authors	:	Poncet-Montange, G.; Assairi, L.; Gelin, M.; Pochet, S.; Labesse, G.
Deposited on	:	2015-11-01
Resolution	:	2.88 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:

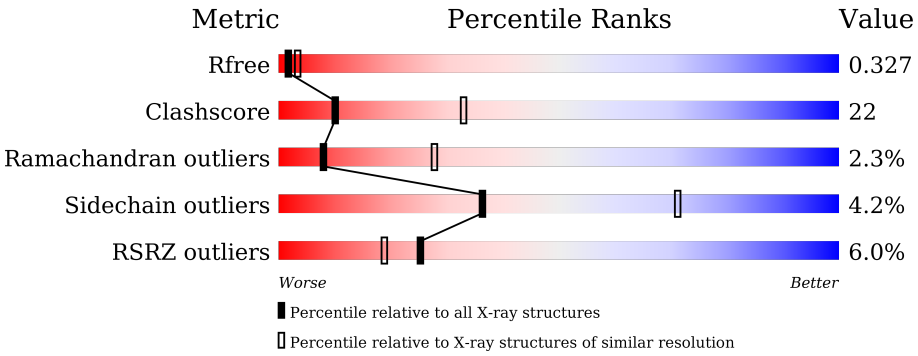
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

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 2.88 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	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (2.90-2.86)

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	272	53% 38% 7%
1	B	272	6% 52% 38% 7%
1	C	272	12% 45% 30% 5% 20%
1	D	272	3% 54% 33% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7671 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 NAD kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			2004	1284	334	377	9			
1	B	254	Total	C	N	O	S	0	0	0
			1971	1269	324	371	7			
1	C	218	Total	C	N	O	S	0	0	0
			1635	1047	278	303	7			
1	D	252	Total	C	N	O	S	0	1	0
			1949	1247	331	364	7			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	252	ASP	PRO	engineered mutation	UNP Q8Y8D7
A	265	LEU	-	expression tag	UNP Q8Y8D7
A	266	GLU	-	expression tag	UNP Q8Y8D7
A	267	HIS	-	expression tag	UNP Q8Y8D7
A	268	HIS	-	expression tag	UNP Q8Y8D7
A	269	HIS	-	expression tag	UNP Q8Y8D7
A	270	HIS	-	expression tag	UNP Q8Y8D7
A	271	HIS	-	expression tag	UNP Q8Y8D7
A	272	HIS	-	expression tag	UNP Q8Y8D7
B	252	ASP	PRO	engineered mutation	UNP Q8Y8D7
B	265	LEU	-	expression tag	UNP Q8Y8D7
B	266	GLU	-	expression tag	UNP Q8Y8D7
B	267	HIS	-	expression tag	UNP Q8Y8D7
B	268	HIS	-	expression tag	UNP Q8Y8D7
B	269	HIS	-	expression tag	UNP Q8Y8D7
B	270	HIS	-	expression tag	UNP Q8Y8D7
B	271	HIS	-	expression tag	UNP Q8Y8D7
B	272	HIS	-	expression tag	UNP Q8Y8D7
C	252	ASP	PRO	engineered mutation	UNP Q8Y8D7
C	265	LEU	-	expression tag	UNP Q8Y8D7
C	266	GLU	-	expression tag	UNP Q8Y8D7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	267	HIS	-	expression tag	UNP Q8Y8D7
C	268	HIS	-	expression tag	UNP Q8Y8D7
C	269	HIS	-	expression tag	UNP Q8Y8D7
C	270	HIS	-	expression tag	UNP Q8Y8D7
C	271	HIS	-	expression tag	UNP Q8Y8D7
C	272	HIS	-	expression tag	UNP Q8Y8D7
D	252	ASP	PRO	engineered mutation	UNP Q8Y8D7
D	265	LEU	-	expression tag	UNP Q8Y8D7
D	266	GLU	-	expression tag	UNP Q8Y8D7
D	267	HIS	-	expression tag	UNP Q8Y8D7
D	268	HIS	-	expression tag	UNP Q8Y8D7
D	269	HIS	-	expression tag	UNP Q8Y8D7
D	270	HIS	-	expression tag	UNP Q8Y8D7
D	271	HIS	-	expression tag	UNP Q8Y8D7
D	272	HIS	-	expression tag	UNP Q8Y8D7

- Molecule 2 is water.

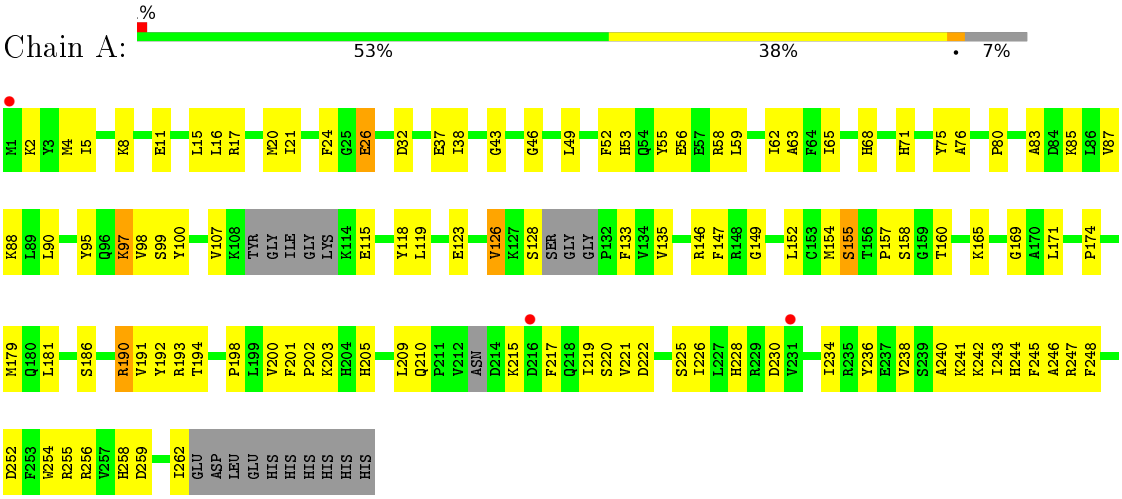
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	47	Total O 47 47	0	0
2	B	33	Total O 33 33	0	0
2	C	19	Total O 19 19	0	0
2	D	13	Total O 13 13	0	0

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.

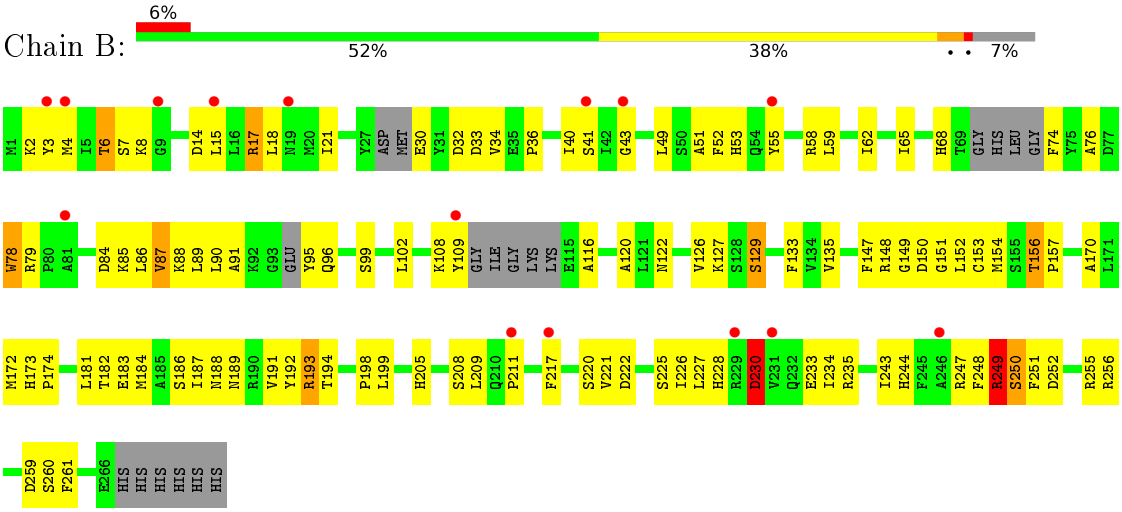
- Molecule 1: NAD kinase 1

Chain A:



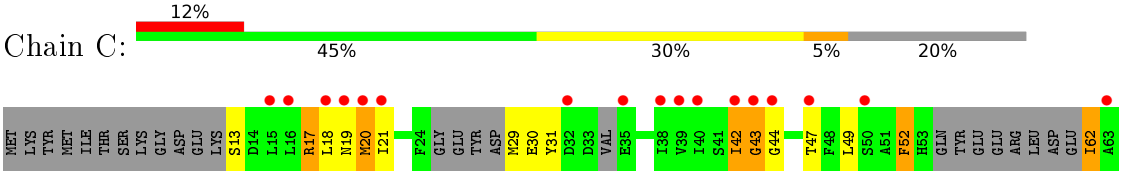
- Molecule 1: NAD kinase 1

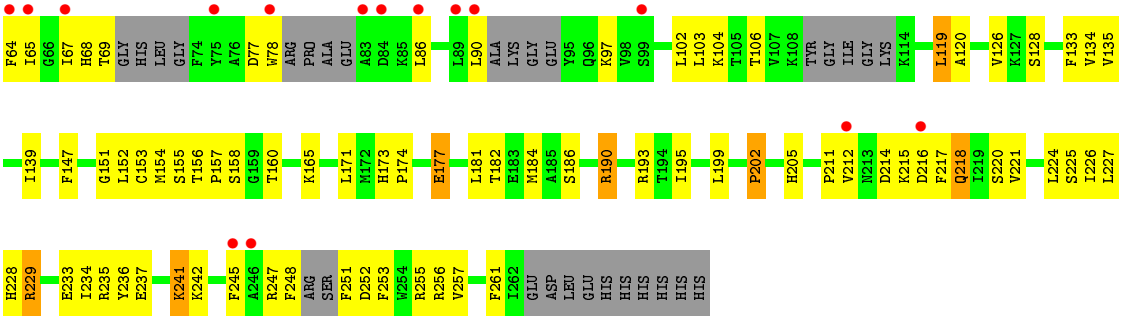
Chain B:



- Molecule 1: NAD kinase 1

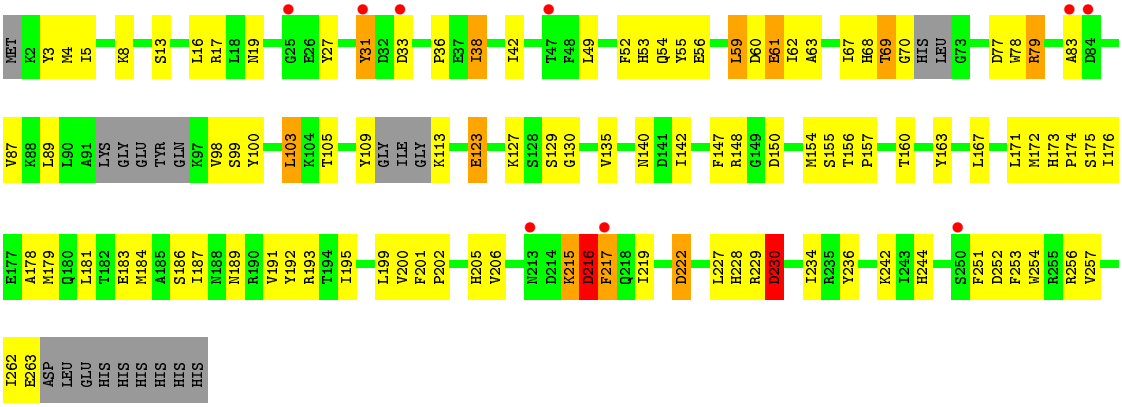
Chain C:





- Molecule 1: NAD kinase 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.22Å 119.66Å 68.62Å 90.00° 100.92° 90.00°	Depositor
Resolution (Å)	18.64 – 2.88 35.04 – 2.88	Depositor EDS
% Data completeness (in resolution range)	97.6 (18.64-2.88) 97.4 (35.04-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	0.70 (at 2.85Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.217 , 0.324 0.219 , 0.327	Depositor DCC
R_{free} test set	755 reflections (3.20%)	DCC
Wilson B-factor (Å^2)	46.4	Xtriage
Anisotropy	0.615	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 96.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.042 for l,-k,h	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	7671	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.40% 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

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	0.52	0/2049	0.68	0/2766
1	B	0.52	1/2016 (0.0%)	0.75	1/2733 (0.0%)
1	C	0.50	0/1667	0.76	2/2260 (0.1%)
1	D	0.52	0/1997	0.76	5/2705 (0.2%)
All	All	0.52	1/7729 (0.0%)	0.74	8/10464 (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
1	B	0	2
1	C	0	2
1	D	0	4
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	78	TRP	C-N	5.61	1.47	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	103	LEU	CA-CB-CG	6.39	130.00	115.30
1	C	119	LEU	CA-CB-CG	-6.30	100.80	115.30
1	C	229	ARG	NE-CZ-NH2	5.59	123.10	120.30
1	D	17	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	D	79	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	D	31	TYR	CB-CG-CD2	5.30	124.18	121.00
1	B	230	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	D	230	ASP	CB-CG-OD1	5.09	122.88	118.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	249	ARG	Peptide
1	B	250	SER	Peptide
1	C	20	MET	Peptide
1	C	42	ILE	Peptide
1	D	215	LYS	Peptide
1	D	216	ASP	Peptide
1	D	67	ILE	Peptide
1	D	89	LEU	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	2004	0	1940	81	0
1	B	1971	0	1869	97	0
1	C	1635	0	1509	82	0
1	D	1949	0	1842	81	0
2	A	47	0	0	4	0
2	B	33	0	0	1	0
2	C	19	0	0	2	0
2	D	13	0	0	3	0
All	All	7671	0	7160	322	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 22.

All (322) 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:C:220:SER:OG	1:C:224:LEU:O	1.91	0.89
1:C:211:PRO:HB3	1:C:217:PHE:HZ	1.37	0.87
1:D:59:LEU:O	1:D:61:GLU:N	2.09	0.86
1:A:169:GLY:O	2:A:301:HOH:O	1.96	0.84
1:C:216:ASP:HB3	1:C:229:ARG:HA	1.56	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:MET:HG2	1:C:30:GLU:H	1.44	0.83
1:B:84:ASP:HA	1:B:87:VAL:HG13	1.60	0.82
1:D:4:MET:HG2	1:D:5:ILE:N	1.96	0.80
1:C:106:THR:HB	1:C:235:ARG:HB3	1.66	0.77
1:D:49:LEU:HD21	1:D:222:ASP:HB3	1.66	0.77
1:C:43:GLY:HA2	1:C:69:THR:H	1.49	0.77
1:D:109:TYR:HB2	1:D:113:LYS:HA	1.67	0.76
1:A:4:MET:HG2	1:A:5:ILE:N	2.01	0.76
1:B:261:PHE:O	1:D:193:ARG:NH2	2.20	0.74
1:D:79:ARG:HH11	1:D:79:ARG:HG3	1.52	0.74
1:A:128:SER:HB3	1:A:217:PHE:HA	1.69	0.74
1:B:4:MET:HB3	1:B:32:ASP:O	1.88	0.74
1:C:214:ASP:OD1	1:C:215:LYS:N	2.24	0.71
1:A:26:GLU:OE2	2:A:302:HOH:O	2.08	0.71
1:B:152:LEU:HD13	1:B:181:LEU:HD11	1.72	0.70
1:B:148:ARG:HG2	1:B:187:ILE:HD12	1.73	0.70
1:C:216:ASP:HB3	1:C:229:ARG:HG3	1.73	0.70
1:A:126:VAL:HG12	1:A:219:ILE:HG12	1.73	0.69
1:C:235:ARG:NH2	1:C:237:GLU:OE1	2.23	0.69
1:B:220:SER:HA	1:B:225:SER:HA	1.73	0.69
1:C:49:LEU:O	1:C:52:PHE:HD2	1.77	0.68
1:D:56:GLU:HA	1:D:59:LEU:HG	1.74	0.68
1:D:68:HIS:HB3	1:D:78:TRP:O	1.94	0.68
1:D:150:ASP:O	2:D:302:HOH:O	2.11	0.67
1:A:53:HIS:ND1	1:A:56:GLU:OE2	2.26	0.67
1:D:160:THR:HG21	1:D:172:MET:HG3	1.78	0.66
1:B:2:LYS:HZ3	1:B:32:ASP:HB2	1.60	0.66
1:B:87:VAL:O	1:B:91:ALA:HB2	1.96	0.65
1:C:177:GLU:O	2:C:301:HOH:O	2.14	0.65
1:B:157:PRO:HB2	1:B:174:PRO:HA	1.79	0.65
1:D:3:TYR:CE1	1:D:31:TYR:HD1	2.16	0.64
1:C:43:GLY:HA2	1:C:69:THR:HG23	1.79	0.64
1:D:79:ARG:HG3	1:D:79:ARG:NH1	2.12	0.64
1:A:98:VAL:O	1:A:244:HIS:HA	1.96	0.63
1:B:85:LYS:HE2	1:B:89:LEU:HD11	1.79	0.63
1:C:29:MET:HG2	1:C:30:GLU:N	2.14	0.63
1:A:16:LEU:HD22	1:A:80:PRO:HB3	1.81	0.62
1:B:250:SER:OG	1:B:251:PHE:N	2.32	0.62
1:B:208:SER:HB2	1:B:235:ARG:HG3	1.80	0.62
1:C:102:LEU:HB2	1:C:241:LYS:HD2	1.81	0.62
1:C:44:GLY:HA3	1:C:68:HIS:HD2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ILE:O	1:C:44:GLY:N	2.33	0.60
1:A:252:ASP:OD2	1:A:255:ARG:HB2	2.01	0.60
1:B:30:GLU:OE1	1:B:30:GLU:N	2.35	0.60
1:B:6:THR:HG23	1:B:41:SER:HA	1.82	0.60
1:C:256:ARG:NH2	2:C:302:HOH:O	2.34	0.60
1:A:146:ARG:HG2	1:A:192:TYR:HD1	1.67	0.59
1:C:247:ARG:HH22	1:C:251:PHE:N	2.01	0.59
1:A:2:LYS:NZ	1:A:32:ASP:OD2	2.26	0.59
1:B:99:SER:OG	1:B:244:HIS:ND1	2.35	0.59
1:D:154:MET:HE1	1:D:181:LEU:HB2	1.84	0.59
1:B:133:PHE:CE2	1:B:151:GLY:HA2	2.38	0.58
1:D:252:ASP:H	1:D:256:ARG:NH2	2.01	0.58
1:A:95:TYR:HB3	1:A:248:PHE:CE1	2.37	0.58
1:B:84:ASP:O	1:B:87:VAL:HG22	2.03	0.58
1:C:235:ARG:HG2	1:C:235:ARG:HH11	1.69	0.58
1:C:119:LEU:HD13	1:C:241:LYS:HZ2	1.68	0.58
1:B:255:ARG:NH1	1:B:259:ASP:OD2	2.36	0.57
1:A:98:VAL:HG21	1:A:247:ARG:CZ	2.34	0.57
1:A:4:MET:SD	1:A:55:TYR:OH	2.56	0.57
1:B:53:HIS:CE1	1:B:222:ASP:HB2	2.39	0.57
1:A:37:GLU:O	1:A:38:ILE:HG12	2.05	0.57
1:A:8:LYS:HB2	1:A:43:GLY:HA3	1.86	0.57
1:B:247:ARG:NH1	1:B:251:PHE:HB3	2.20	0.57
1:B:52:PHE:HD2	1:B:53:HIS:HD2	1.51	0.57
1:D:16:LEU:HA	1:D:19:ASN:OD1	2.04	0.57
1:C:202:PRO:HD2	1:C:205:HIS:CG	2.40	0.56
1:C:49:LEU:O	1:C:52:PHE:HB3	2.05	0.56
1:C:202:PRO:HB3	1:D:176:ILE:HG12	1.87	0.56
1:B:182:THR:HG22	1:B:198:PRO:HB3	1.86	0.56
1:B:33:ASP:O	1:B:55:TYR:OH	2.17	0.56
1:A:68:HIS:ND1	1:A:71:HIS:O	2.39	0.56
1:A:17:ARG:O	1:A:21:ILE:HG13	2.05	0.56
1:B:252:ASP:HB3	1:B:255:ARG:HB3	1.86	0.56
1:B:120:ALA:HB2	1:B:221:VAL:HG13	1.87	0.56
1:D:3:TYR:CZ	1:D:31:TYR:HB2	2.40	0.56
1:B:135:VAL:HG11	1:B:209:LEU:HB3	1.86	0.56
1:D:173:HIS:CE1	1:D:175:SER:H	2.24	0.56
1:D:3:TYR:CE2	1:D:31:TYR:HB2	2.41	0.56
1:A:68:HIS:HB2	1:A:76:ALA:CB	2.37	0.55
1:B:74:PHE:CE1	1:B:256:ARG:HG2	2.41	0.55
1:A:99:SER:HB3	1:A:242:LYS:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:PHE:HD2	1:B:194:THR:HG21	1.72	0.55
1:C:62:ILE:HD12	1:C:64:PHE:HE2	1.71	0.55
1:A:190:ARG:HG2	1:A:191:VAL:N	2.22	0.55
1:D:135:VAL:HG12	1:D:147:PHE:HB3	1.88	0.55
1:A:205:HIS:CE1	1:B:173:HIS:CD2	2.94	0.55
1:B:188:ASN:HA	1:B:192:TYR:O	2.06	0.55
1:C:211:PRO:HB3	1:C:217:PHE:CZ	2.28	0.55
1:A:83:ALA:O	1:A:87:VAL:HG23	2.07	0.55
1:A:202:PRO:HG2	1:A:205:HIS:CD2	2.42	0.54
1:B:68:HIS:CE1	1:B:79:ARG:HG2	2.43	0.54
1:C:97:LYS:HA	1:C:245:PHE:O	2.07	0.54
1:D:216:ASP:HB2	1:D:217:PHE:CD1	2.41	0.54
1:B:95:TYR:HB3	1:B:248:PHE:CE2	2.41	0.54
1:D:99:SER:O	1:D:100:TYR:HD1	1.90	0.54
1:B:90:LEU:HD12	1:B:248:PHE:HZ	1.72	0.54
1:C:65:ILE:HD12	1:C:248:PHE:HE1	1.72	0.54
1:C:43:GLY:CA	1:C:69:THR:HG23	2.37	0.54
1:A:220:SER:HA	1:A:225:SER:HA	1.90	0.54
1:B:199:LEU:HG	2:B:315:HOH:O	2.07	0.54
1:B:76:ALA:O	1:B:256:ARG:NH1	2.32	0.54
1:D:217:PHE:CD2	1:D:234:ILE:HD11	2.43	0.54
1:D:38:ILE:HG13	1:D:63:ALA:HB3	1.89	0.53
1:D:54:GLN:HB3	1:D:55:TYR:CD1	2.42	0.53
1:A:90:LEU:HD13	1:A:248:PHE:HZ	1.74	0.53
1:D:83:ALA:O	1:D:87:VAL:HG23	2.08	0.53
1:A:209:LEU:HD11	1:A:236:TYR:HE2	1.74	0.53
1:A:154:MET:CE	1:A:181:LEU:HB2	2.39	0.52
1:A:5:ILE:HB	1:A:17:ARG:HD2	1.91	0.52
1:B:2:LYS:HG3	1:B:32:ASP:HB2	1.90	0.52
1:B:109:TYR:HD1	1:B:230:ASP:OD2	1.92	0.52
1:B:2:LYS:HG2	1:B:36:PRO:HA	1.91	0.52
1:B:2:LYS:CG	1:B:32:ASP:HB2	2.40	0.52
1:C:104:LYS:NZ	1:C:106:THR:OG1	2.33	0.51
1:C:157:PRO:HB2	1:C:174:PRO:HA	1.91	0.51
1:A:119:LEU:HD11	1:A:241:LYS:HD3	1.93	0.51
1:B:8:LYS:HB2	1:B:43:GLY:HA3	1.92	0.51
1:A:157:PRO:HB2	1:A:174:PRO:HA	1.93	0.51
1:C:241:LYS:HG2	1:C:242:LYS:N	2.25	0.51
1:C:49:LEU:O	1:C:52:PHE:CD2	2.62	0.51
1:B:74:PHE:HA	1:B:256:ARG:HD3	1.92	0.51
1:B:126:VAL:HG12	1:B:133:PHE:HE1	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:LEU:HA	1:C:21:ILE:HG13	1.92	0.51
1:A:123:GLU:HA	1:A:155:SER:HA	1.93	0.50
1:C:147:PHE:CE1	1:C:186:SER:HB3	2.45	0.50
1:D:179:MET:O	1:D:200:VAL:HA	2.11	0.50
1:A:97:LYS:HA	1:A:245:PHE:O	2.11	0.50
1:B:226:ILE:HG13	1:B:228:HIS:NE2	2.26	0.50
1:D:253:PHE:O	1:D:257:VAL:HG23	2.11	0.50
1:A:56:GLU:HA	1:A:59:LEU:HG	1.92	0.50
1:B:52:PHE:CD2	1:B:53:HIS:HD2	2.28	0.50
1:D:252:ASP:H	1:D:256:ARG:HH22	1.59	0.50
1:A:152:LEU:HB3	1:A:181:LEU:HD11	1.93	0.50
1:A:203:LYS:HG3	1:A:238:VAL:HG11	1.92	0.50
1:B:193:ARG:NE	1:C:193:ARG:HD3	2.27	0.50
1:D:227:LEU:HD11	1:D:229:ARG:NH1	2.27	0.50
1:A:198:PRO:HD2	1:B:170:ALA:HA	1.94	0.50
1:A:52:PHE:CD1	1:A:243:ILE:HD12	2.47	0.49
1:D:4:MET:HE3	1:D:33:ASP:HA	1.94	0.49
1:A:16:LEU:O	1:A:20:MET:HG3	2.12	0.49
1:A:165:LYS:HD2	1:A:171:LEU:HD21	1.94	0.49
1:B:6:THR:HG21	1:B:51:ALA:HB2	1.94	0.49
1:C:171:LEU:HB2	1:D:199:LEU:HD23	1.94	0.49
1:B:153:CYS:O	1:B:181:LEU:HA	2.13	0.49
1:D:127:LYS:O	1:D:217:PHE:HA	2.12	0.49
1:D:192:TYR:O	2:D:303:HOH:O	2.20	0.49
1:B:252:ASP:O	1:B:255:ARG:HB3	2.11	0.49
1:B:2:LYS:NZ	1:B:32:ASP:HB2	2.26	0.49
1:A:100:TYR:HB3	2:A:311:HOH:O	2.11	0.49
1:D:157:PRO:HB2	1:D:174:PRO:HA	1.94	0.49
1:C:67:ILE:HD13	1:C:78:TRP:HB3	1.95	0.49
1:D:54:GLN:HB3	1:D:55:TYR:CE1	2.47	0.49
1:B:74:PHE:CD1	1:B:256:ARG:HG2	2.48	0.49
1:C:18:LEU:HA	1:C:21:ILE:CG1	2.43	0.49
1:C:104:LYS:HE3	1:C:235:ARG:NH1	2.28	0.49
1:D:173:HIS:HB2	1:D:254:TRP:CZ2	2.48	0.49
1:D:99:SER:HB3	1:D:242:LYS:HD2	1.93	0.49
1:B:260:SER:O	1:D:189:ASN:HB2	2.12	0.48
1:A:65:ILE:HG12	1:A:246:ALA:HB3	1.96	0.48
1:B:78:TRP:CE2	1:B:86:LEU:HD13	2.48	0.48
1:C:18:LEU:O	1:C:18:LEU:HD23	2.14	0.48
1:C:252:ASP:HB3	1:C:255:ARG:HB3	1.93	0.48
1:C:158:SER:HA	1:C:174:PRO:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:VAL:HG21	1:C:234:ILE:HD13	1.95	0.48
1:D:219:ILE:HD12	1:D:228:HIS:CD2	2.49	0.48
1:B:126:VAL:HG12	1:B:133:PHE:CE1	2.48	0.48
1:A:154:MET:SD	1:A:179:MET:HB2	2.53	0.48
1:A:205:HIS:HE1	1:B:173:HIS:CD2	2.31	0.48
1:B:2:LYS:HD3	1:B:32:ASP:OD2	2.13	0.48
1:C:147:PHE:CG	1:C:152:LEU:HD21	2.48	0.48
1:C:218:GLN:HG3	1:C:227:LEU:HD12	1.95	0.48
1:C:65:ILE:HD13	1:C:86:LEU:HD11	1.95	0.48
1:B:33:ASP:OD1	1:B:34:VAL:HG13	2.14	0.47
1:C:44:GLY:HA2	1:C:68:HIS:HB2	1.96	0.47
1:D:154:MET:SD	1:D:179:MET:HB2	2.54	0.47
1:A:226:ILE:HB	1:A:228:HIS:HE1	1.79	0.47
1:B:65:ILE:HD11	1:B:86:LEU:HD11	1.96	0.47
1:B:127:LYS:HG2	1:B:150:ASP:O	2.15	0.47
1:D:202:PRO:HG2	1:D:205:HIS:CD2	2.49	0.47
1:A:135:VAL:HG21	1:A:209:LEU:HB3	1.96	0.47
1:A:4:MET:CG	1:A:5:ILE:N	2.76	0.47
1:B:152:LEU:HD23	1:B:183:GLU:HA	1.96	0.47
1:D:103:LEU:HD23	1:D:156:THR:HG22	1.95	0.47
1:A:24:PHE:CD1	1:A:87:VAL:HG13	2.50	0.47
1:C:62:ILE:HD12	1:C:64:PHE:CE2	2.49	0.47
1:D:8:LYS:HB3	1:D:13:SER:OG	2.14	0.47
1:D:140:ASN:HA	1:D:206:VAL:HG12	1.96	0.46
1:B:252:ASP:HB3	1:B:255:ARG:CB	2.44	0.46
1:C:77:ASP:HB3	1:C:251:PHE:CE1	2.50	0.46
1:D:167:LEU:HD23	1:D:167:LEU:HA	1.74	0.46
1:C:119:LEU:HD13	1:C:241:LYS:NZ	2.31	0.46
1:C:226:ILE:HG13	1:C:226:ILE:O	2.15	0.46
1:D:179:MET:HG3	1:D:201:PHE:HB2	1.97	0.46
1:D:262:ILE:HG22	1:D:263:GLU:N	2.30	0.46
1:A:146:ARG:HG2	1:A:192:TYR:CD1	2.49	0.46
1:B:52:PHE:CE1	1:B:59:LEU:HD11	2.51	0.46
1:C:156:THR:O	1:C:160:THR:HG23	2.16	0.46
1:B:99:SER:HG	1:B:244:HIS:CE1	2.32	0.46
1:B:147:PHE:HE2	1:B:186:SER:HB3	1.80	0.46
1:B:58:ARG:O	1:B:62:ILE:HG13	2.16	0.46
1:C:247:ARG:HH12	1:C:251:PHE:N	2.13	0.46
1:D:69:THR:HG23	1:D:70:GLY:H	1.80	0.46
1:A:240:ALA:N	2:A:305:HOH:O	2.31	0.45
1:D:147:PHE:HE2	1:D:183:GLU:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:PHE:HE2	1:D:53:HIS:CE1	2.34	0.45
1:A:154:MET:HE1	1:A:181:LEU:HB2	1.97	0.45
1:A:147:PHE:CE2	1:A:186:SER:HB2	2.51	0.45
1:A:255:ARG:O	1:A:258:HIS:HB3	2.16	0.45
1:B:151:GLY:O	1:B:184:MET:HB2	2.16	0.45
1:A:133:PHE:HB3	1:A:149:GLY:O	2.16	0.45
1:A:52:PHE:HD1	1:A:243:ILE:HD12	1.80	0.45
1:D:251:PHE:HD1	1:D:252:ASP:N	2.13	0.45
1:D:4:MET:HE1	1:D:55:TYR:CZ	2.52	0.45
1:A:157:PRO:HA	1:A:160:THR:HG23	1.99	0.45
1:B:233:GLU:CD	1:B:235:ARG:HD3	2.37	0.45
1:D:148:ARG:O	1:D:187:ILE:HG12	2.16	0.45
1:D:215:LYS:HB3	1:D:230:ASP:HA	1.99	0.45
1:B:147:PHE:CD2	1:B:194:THR:HG21	2.50	0.45
1:C:29:MET:CG	1:C:30:GLU:H	2.19	0.45
1:A:226:ILE:HB	1:A:228:HIS:CE1	2.52	0.44
1:C:171:LEU:HB2	1:D:199:LEU:CD2	2.47	0.44
1:A:200:VAL:HG23	1:B:170:ALA:HB1	1.99	0.44
1:B:108:LYS:HG3	1:B:109:TYR:H	1.81	0.44
1:C:205:HIS:CE1	1:D:254:TRP:HE1	2.36	0.44
1:C:165:LYS:HD3	1:C:261:PHE:CZ	2.53	0.44
1:A:85:LYS:HA	1:A:88:LYS:HE2	1.99	0.44
1:D:98:VAL:O	1:D:244:HIS:HA	2.17	0.44
1:B:17:ARG:O	1:B:21:ILE:HG13	2.16	0.44
1:C:202:PRO:HB3	1:D:176:ILE:CG1	2.46	0.44
1:A:200:VAL:HB	1:B:172:MET:HG2	2.00	0.44
1:A:53:HIS:NE2	1:A:222:ASP:OD2	2.50	0.44
1:C:216:ASP:CB	1:C:229:ARG:HA	2.38	0.44
1:C:153:CYS:O	1:C:181:LEU:HA	2.18	0.44
1:B:15:LEU:HA	1:B:15:LEU:HD12	1.64	0.44
1:D:100:TYR:HH	1:D:251:PHE:HE2	1.63	0.44
1:D:178:ALA:HB1	1:D:200:VAL:HG12	2.00	0.44
1:D:4:MET:HE3	1:D:4:MET:HB2	1.91	0.44
1:B:189:ASN:O	1:B:191:VAL:N	2.47	0.43
1:D:123:GLU:HA	1:D:155:SER:HA	2.00	0.43
1:A:107:VAL:O	1:A:115:GLU:HB2	2.18	0.43
1:A:52:PHE:HD2	1:A:53:HIS:CD2	2.35	0.43
1:B:88:LYS:O	1:B:91:ALA:HB3	2.18	0.43
1:A:126:VAL:HG11	1:A:234:ILE:HD13	2.00	0.43
1:A:258:HIS:ND1	1:A:262:ILE:HB	2.33	0.43
1:A:46:GLY:O	1:A:49:LEU:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:GLY:O	1:C:184:MET:HB2	2.18	0.43
1:A:118:TYR:OH	1:A:228:HIS:NE2	2.43	0.43
1:B:18:LEU:HD12	1:B:21:ILE:HB	2.00	0.43
1:B:99:SER:OG	1:B:244:HIS:CE1	2.71	0.43
1:D:5:ILE:HG21	1:D:42:ILE:HD11	2.01	0.43
1:B:247:ARG:HH12	1:B:251:PHE:HB3	1.83	0.43
1:C:134:VAL:O	1:C:212:VAL:HG13	2.18	0.43
1:B:122:ASN:O	1:B:156:THR:HG23	2.18	0.43
1:C:171:LEU:HD12	1:D:199:LEU:HD21	2.00	0.43
1:B:108:LYS:HG3	1:B:109:TYR:N	2.34	0.43
1:C:220:SER:HB2	1:C:225:SER:HA	2.00	0.43
1:D:105:THR:HG1	1:D:236:TYR:HE1	1.65	0.43
1:B:109:TYR:OH	1:B:116:ALA:HB3	2.19	0.43
1:C:195:ILE:HD12	1:C:195:ILE:HA	1.90	0.42
1:B:102:LEU:HD21	1:B:243:ILE:HB	2.01	0.42
1:B:40:ILE:HG12	1:B:65:ILE:CG2	2.49	0.42
1:C:252:ASP:OD2	1:D:142:ILE:HD12	2.19	0.42
1:B:49:LEU:HA	1:B:49:LEU:HD23	1.83	0.42
1:A:90:LEU:HD12	1:A:90:LEU:HA	1.87	0.42
1:B:109:TYR:CD1	1:B:230:ASP:OD2	2.70	0.42
1:B:3:TYR:OH	1:B:21:ILE:HG23	2.19	0.42
1:D:4:MET:HE3	1:D:36:PRO:HG3	2.01	0.42
1:A:11:GLU:O	1:A:15:LEU:HB2	2.19	0.42
1:A:75:TYR:OH	1:A:158:SER:HB2	2.19	0.42
1:B:6:THR:CG2	1:B:41:SER:HA	2.48	0.42
1:B:249:ARG:O	1:B:250:SER:HB2	2.19	0.42
1:B:52:PHE:HD2	1:B:53:HIS:CD2	2.33	0.42
1:B:154:MET:CE	1:B:181:LEU:HB2	2.49	0.42
1:B:209:LEU:N	1:B:234:ILE:O	2.39	0.42
1:A:259:ASP:O	1:C:190:ARG:HD2	2.20	0.42
1:A:179:MET:HG3	1:A:201:PHE:HB2	2.02	0.42
1:B:211:PRO:HB3	1:B:217:PHE:HZ	1.85	0.42
1:C:86:LEU:O	1:C:90:LEU:N	2.47	0.42
1:A:193:ARG:CZ	1:D:193:ARG:HD3	2.50	0.42
1:C:235:ARG:NH1	1:C:235:ARG:HG2	2.32	0.42
1:B:133:PHE:HB3	1:B:149:GLY:O	2.20	0.41
1:C:199:LEU:HD23	1:D:171:LEU:HB2	2.01	0.41
1:A:24:PHE:CE1	1:A:87:VAL:HG13	2.55	0.41
1:B:152:LEU:HB3	1:B:181:LEU:HD11	2.02	0.41
1:A:254:TRP:HE1	1:B:205:HIS:CE1	2.38	0.41
1:D:215:LYS:CB	1:D:230:ASP:HA	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:PRO:O	1:D:62:ILE:HG12	2.20	0.41
1:C:128:SER:HB3	1:C:133:PHE:HB2	2.02	0.41
1:D:4:MET:CG	1:D:5:ILE:N	2.77	0.41
1:D:202:PRO:HD2	1:D:205:HIS:CG	2.56	0.41
1:D:4:MET:CE	1:D:36:PRO:HG3	2.50	0.41
1:C:154:MET:HG2	1:C:236:TYR:HB3	2.02	0.41
1:C:120:ALA:HB2	1:C:221:VAL:HG13	2.01	0.41
1:D:167:LEU:HD11	1:D:184:MET:HG2	2.02	0.41
1:B:217:PHE:O	1:B:227:LEU:HD12	2.21	0.41
1:D:195:ILE:HG21	1:D:199:LEU:HD11	2.02	0.41
1:A:38:ILE:HD13	1:A:63:ALA:HB3	2.03	0.41
1:D:4:MET:HA	1:D:31:TYR:CE1	2.55	0.41
1:A:215:LYS:NZ	1:A:230:ASP:OD1	2.45	0.41
1:C:227:LEU:HD23	1:C:228:HIS:N	2.35	0.41
1:C:139:ILE:HD13	1:D:254:TRP:HB3	2.03	0.40
1:C:17:ARG:C	1:C:19:ASN:H	2.23	0.40
1:A:118:TYR:CG	1:A:221:VAL:HG21	2.56	0.40
1:D:173:HIS:CE1	1:D:175:SER:HG	2.39	0.40
1:A:5:ILE:HB	1:A:17:ARG:HG3	2.03	0.40
1:A:38:ILE:HG21	1:A:90:LEU:HD21	2.03	0.40
1:A:62:ILE:HD13	1:A:62:ILE:HG21	1.91	0.40
1:C:13:SER:OG	1:C:42:ILE:HG12	2.21	0.40
1:C:158:SER:HB3	1:C:174:PRO:HB3	2.03	0.40
1:C:247:ARG:CZ	1:C:251:PHE:CD2	3.04	0.40
1:C:253:PHE:O	1:C:257:VAL:HG23	2.21	0.40
1:B:53:HIS:HE1	1:B:222:ASP:HB2	1.84	0.40
1:C:103:LEU:HB3	1:C:120:ALA:HB3	2.04	0.40
1:C:173:HIS:ND1	1:C:174:PRO:HD2	2.35	0.40
1:D:217:PHE:HD2	1:D:234:ILE:HD11	1.87	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	245/272 (90%)	221 (90%)	24 (10%)	0	100 100
1	B	244/272 (90%)	218 (89%)	23 (9%)	3 (1%)	16 46
1	C	200/272 (74%)	172 (86%)	21 (10%)	7 (4%)	4 17
1	D	245/272 (90%)	209 (85%)	25 (10%)	11 (4%)	3 11
All	All	934/1088 (86%)	820 (88%)	93 (10%)	21 (2%)	8 29

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	129	SER
1	C	17	ARG
1	C	43	GLY
1	C	241	LYS
1	D	60	ASP
1	D	61	GLU
1	D	216	ASP
1	D	217	PHE
1	D	130	GLY
1	D	222	ASP
1	D	230	ASP
1	B	249	ARG
1	C	177	GLU
1	C	190	ARG
1	D	59	LEU
1	D	163	TYR
1	B	17	ARG
1	D	27	TYR
1	C	31	TYR
1	D	191	VAL
1	C	202	PRO

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	215/237 (91%)	206 (96%)	9 (4%)	36	71
1	B	206/237 (87%)	197 (96%)	9 (4%)	35	69
1	C	165/237 (70%)	156 (94%)	9 (6%)	27	59
1	D	202/237 (85%)	196 (97%)	6 (3%)	48	81
All	All	788/948 (83%)	755 (96%)	33 (4%)	36	71

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	58	ARG
1	A	97	LYS
1	A	126	VAL
1	A	155	SER
1	A	190	ARG
1	A	194	THR
1	A	210	GLN
1	A	256	ARG
1	B	6	THR
1	B	7	SER
1	B	14	ASP
1	B	87	VAL
1	B	96	GLN
1	B	129	SER
1	B	156	THR
1	B	193	ARG
1	B	230	ASP
1	C	20	MET
1	C	47	THR
1	C	52	PHE
1	C	62	ILE
1	C	135	VAL
1	C	155	SER
1	C	182	THR
1	C	218	GLN
1	C	233	GLU
1	D	38	ILE
1	D	69	THR
1	D	77	ASP
1	D	123	GLU
1	D	129	SER
1	D	186	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	HIS
1	C	68	HIS
1	C	140	ASN

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

There are no ligands in this entry.

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	253/272 (93%)	-0.07	3 (1%) 81 79	15, 48, 94, 131	14 (5%)
1	B	254/272 (93%)	0.22	15 (5%) 26 20	12, 56, 117, 169	10 (3%)
1	C	218/272 (80%)	0.54	32 (14%) 3 2	26, 73, 129, 157	4 (1%)
1	D	252/272 (92%)	0.23	9 (3%) 46 40	19, 66, 113, 149	10 (3%)
All	All	977/1088 (89%)	0.22	59 (6%) 25 19	12, 60, 117, 169	38 (3%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	47	THR	5.7
1	C	63	ALA	5.2
1	C	40	ILE	5.1
1	D	213	ASN	5.0
1	C	42	ILE	4.7
1	D	250	SER	4.1
1	C	44	GLY	3.8
1	D	217	PHE	3.8
1	C	15	LEU	3.8
1	C	43	GLY	3.5
1	C	99	SER	3.4
1	C	83	ALA	3.4
1	C	86	LEU	3.4
1	C	64	PHE	3.3
1	B	217	PHE	3.3
1	C	38	ILE	3.3
1	C	32	ASP	3.3
1	B	231	VAL	3.2
1	C	75	TYR	3.2
1	C	16	LEU	3.1
1	C	20	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	67	ILE	3.1
1	B	15	LEU	3.0
1	C	245	PHE	3.0
1	B	55	TYR	3.0
1	B	3	TYR	3.0
1	B	4	MET	3.0
1	D	31	TYR	2.8
1	B	81	ALA	2.7
1	C	84	ASP	2.7
1	A	216	ASP	2.6
1	C	78	TRP	2.6
1	C	21	ILE	2.6
1	B	19	ASN	2.5
1	D	33	ASP	2.5
1	A	231	VAL	2.5
1	C	47	THR	2.5
1	D	25	GLY	2.5
1	C	90	LEU	2.4
1	B	229	ARG	2.4
1	D	84	ASP	2.4
1	B	41	SER	2.4
1	C	246	ALA	2.4
1	D	83	ALA	2.4
1	C	216	ASP	2.4
1	C	35	GLU	2.3
1	C	89	LEU	2.3
1	C	212	VAL	2.3
1	C	18	LEU	2.2
1	C	50	SER	2.2
1	B	109	TYR	2.2
1	B	211	PRO	2.1
1	B	246	ALA	2.1
1	B	43	GLY	2.1
1	C	39	VAL	2.1
1	C	19	ASN	2.1
1	C	65	ILE	2.1
1	A	1	MET	2.0
1	B	9	GLY	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.