Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2023 – 12:37 PM JST

PDB ID	:	5DBU
Title	:	Crystal structure of 2-deoxyribose-5-phosphate aldolase (1-220) from Streptococcus suis
Authors	:	Cao, T.-P.; Choi, J.M.; Lee, S.H.
Deposited on	:	2015-08-22
Resolution	:	2.80 Å(reported)

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

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

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

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

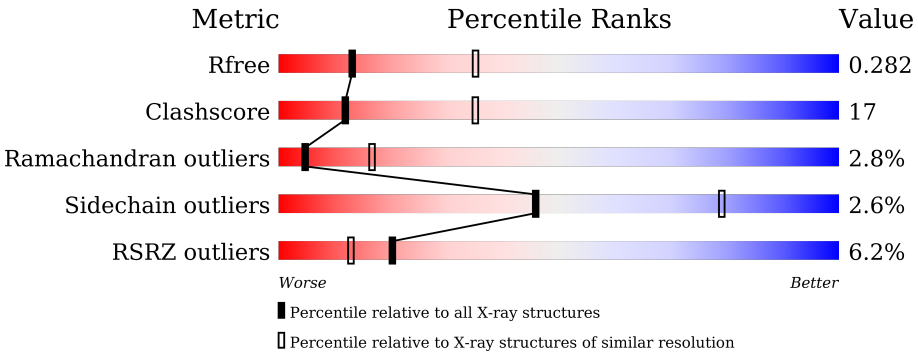
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	223	73% 22% 5%
1	B	223	6% 73% 19% 6%
1	C	223	74% 18% 5%
1	D	223	8% 74% 20% 5%
1	E	223	74% 19% 6%
1	F	223	8% 60% 27% 6% 6%

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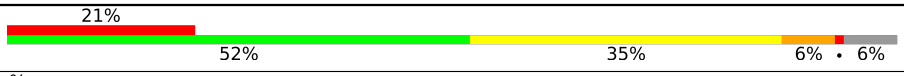
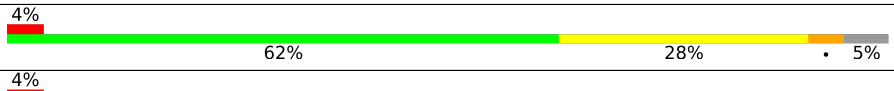
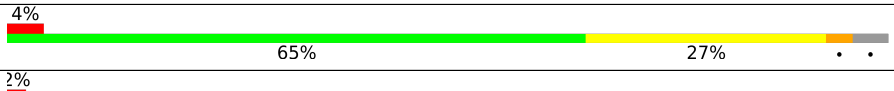
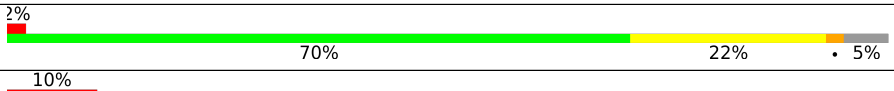
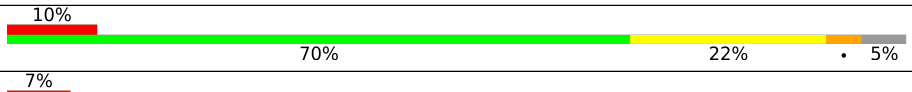
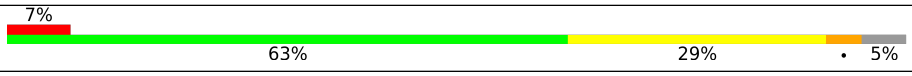
Mol	Chain	Length	Quality of chain
1	G	223	
1	H	223	
1	I	223	
1	J	223	
1	K	223	
1	L	223	
1	M	223	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 20084 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 Deoxyribose-phosphate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1544	971	251	313	9			
1	B	210	Total	C	N	O	S	0	0	0
			1536	966	250	312	8			
1	C	211	Total	C	N	O	S	0	0	0
			1544	971	251	313	9			
1	D	212	Total	C	N	O	S	0	0	0
			1552	975	253	315	9			
1	E	209	Total	C	N	O	S	0	0	0
			1527	960	248	311	8			
1	F	210	Total	C	N	O	S	0	0	0
			1536	966	250	312	8			
1	G	210	Total	C	N	O	S	0	0	0
			1536	966	250	312	8			
1	H	211	Total	C	N	O	S	0	0	0
			1544	971	251	313	9			
1	I	211	Total	C	N	O	S	0	0	0
			1544	971	251	313	9			
1	J	214	Total	C	N	O	S	0	0	0
			1561	980	255	317	9			
1	K	212	Total	C	N	O	S	0	0	0
			1552	975	253	315	9			
1	L	212	Total	C	N	O	S	0	0	0
			1552	975	253	315	9			
1	M	212	Total	C	N	O	S	0	0	0
			1552	975	253	315	9			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP D5AHU8
A	-1	SER	-	expression tag	UNP D5AHU8
A	0	HIS	-	expression tag	UNP D5AHU8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP D5AHU8
B	-1	SER	-	expression tag	UNP D5AHU8
B	0	HIS	-	expression tag	UNP D5AHU8
C	-2	GLY	-	expression tag	UNP D5AHU8
C	-1	SER	-	expression tag	UNP D5AHU8
C	0	HIS	-	expression tag	UNP D5AHU8
D	-2	GLY	-	expression tag	UNP D5AHU8
D	-1	SER	-	expression tag	UNP D5AHU8
D	0	HIS	-	expression tag	UNP D5AHU8
E	-2	GLY	-	expression tag	UNP D5AHU8
E	-1	SER	-	expression tag	UNP D5AHU8
E	0	HIS	-	expression tag	UNP D5AHU8
F	-2	GLY	-	expression tag	UNP D5AHU8
F	-1	SER	-	expression tag	UNP D5AHU8
F	0	HIS	-	expression tag	UNP D5AHU8
G	-2	GLY	-	expression tag	UNP D5AHU8
G	-1	SER	-	expression tag	UNP D5AHU8
G	0	HIS	-	expression tag	UNP D5AHU8
H	-2	GLY	-	expression tag	UNP D5AHU8
H	-1	SER	-	expression tag	UNP D5AHU8
H	0	HIS	-	expression tag	UNP D5AHU8
I	-2	GLY	-	expression tag	UNP D5AHU8
I	-1	SER	-	expression tag	UNP D5AHU8
I	0	HIS	-	expression tag	UNP D5AHU8
J	-2	GLY	-	expression tag	UNP D5AHU8
J	-1	SER	-	expression tag	UNP D5AHU8
J	0	HIS	-	expression tag	UNP D5AHU8
K	-2	GLY	-	expression tag	UNP D5AHU8
K	-1	SER	-	expression tag	UNP D5AHU8
K	0	HIS	-	expression tag	UNP D5AHU8
L	-2	GLY	-	expression tag	UNP D5AHU8
L	-1	SER	-	expression tag	UNP D5AHU8
L	0	HIS	-	expression tag	UNP D5AHU8
M	-2	GLY	-	expression tag	UNP D5AHU8
M	-1	SER	-	expression tag	UNP D5AHU8
M	0	HIS	-	expression tag	UNP D5AHU8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	3	Total O 3 3	0	0

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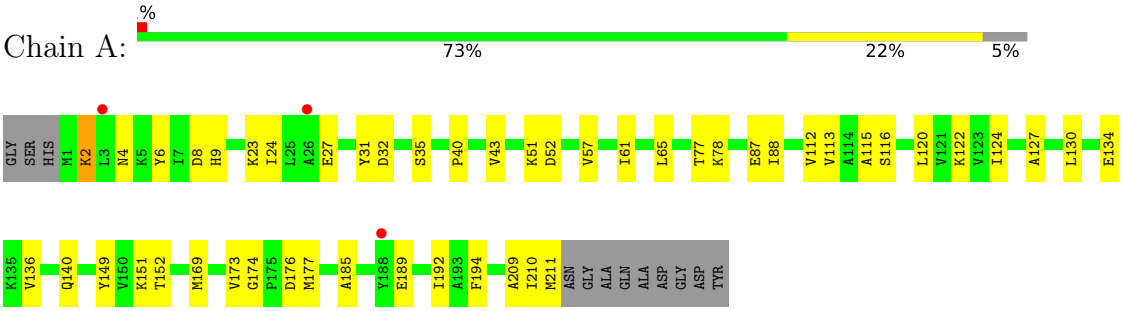
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total O 1 1	0	0

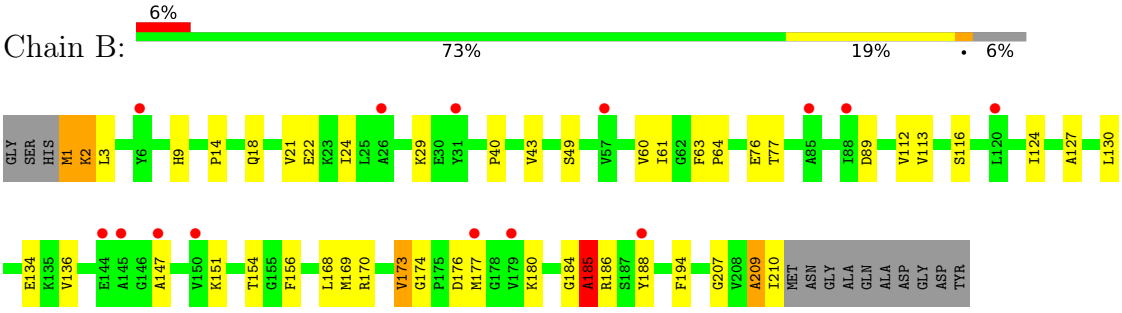
3 Residue-property plots (i)

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

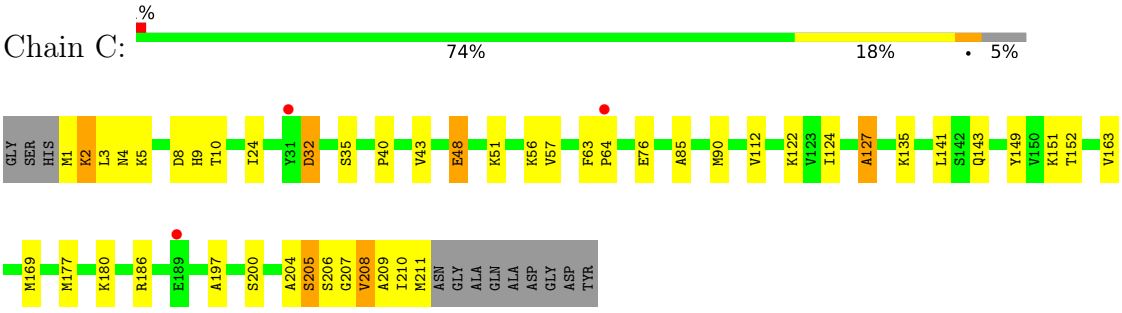
• Molecule 1: Deoxyribose-phosphate aldolase



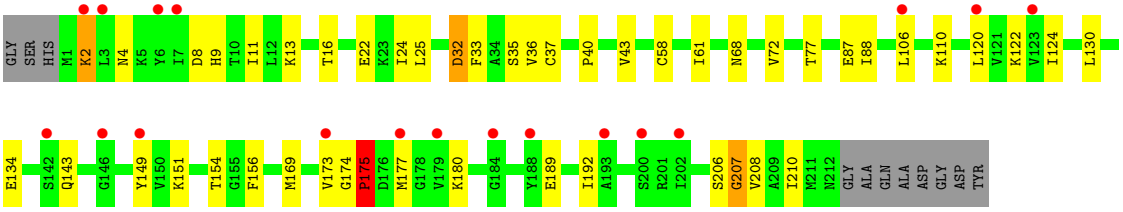
• Molecule 1: Deoxyribose-phosphate aldolase



• Molecule 1: Deoxyribose-phosphate aldolase

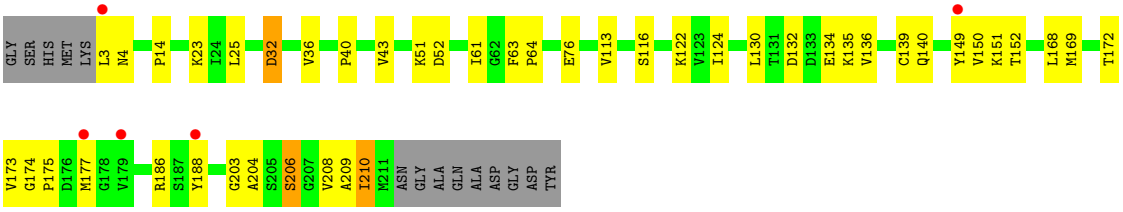


• Molecule 1: Deoxyribose-phosphate aldolase



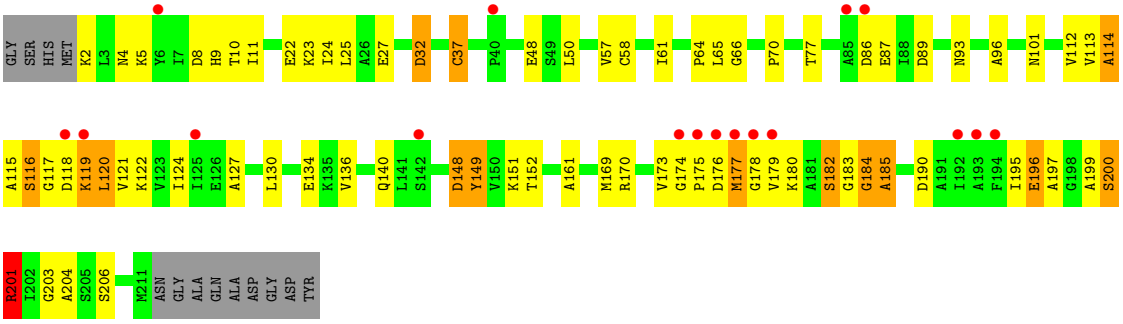
• Molecule 1: Deoxyribose-phosphate aldolase

Chain E:



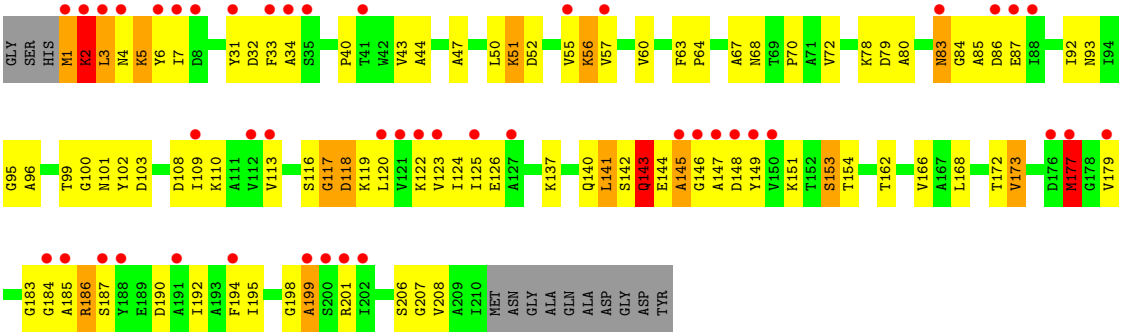
• Molecule 1: Deoxyribose-phosphate aldolase

Chain F:



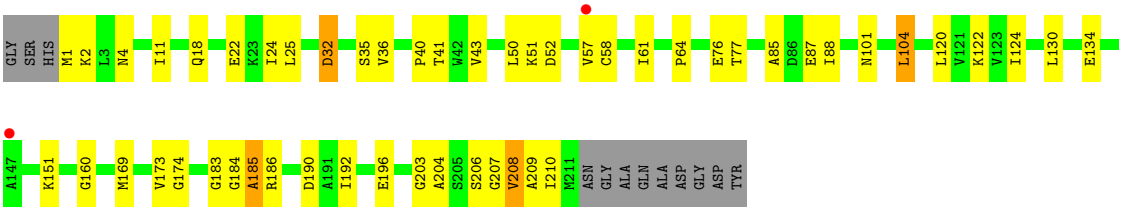
• Molecule 1: Deoxyribose-phosphate aldolase

Chain G:



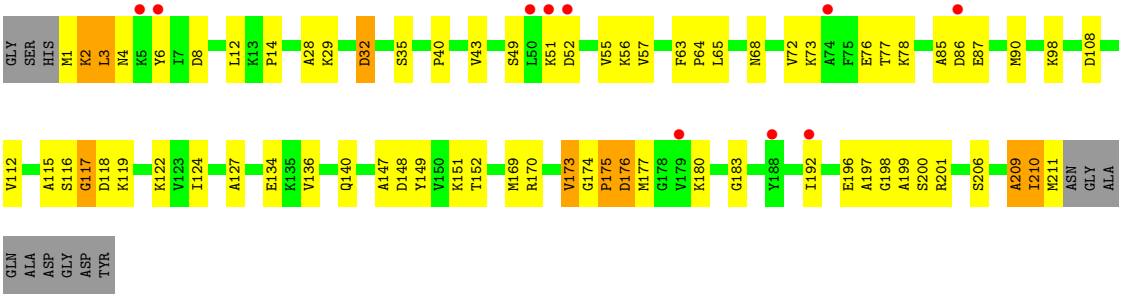
• Molecule 1: Deoxyribose-phosphate aldolase

Chain H:



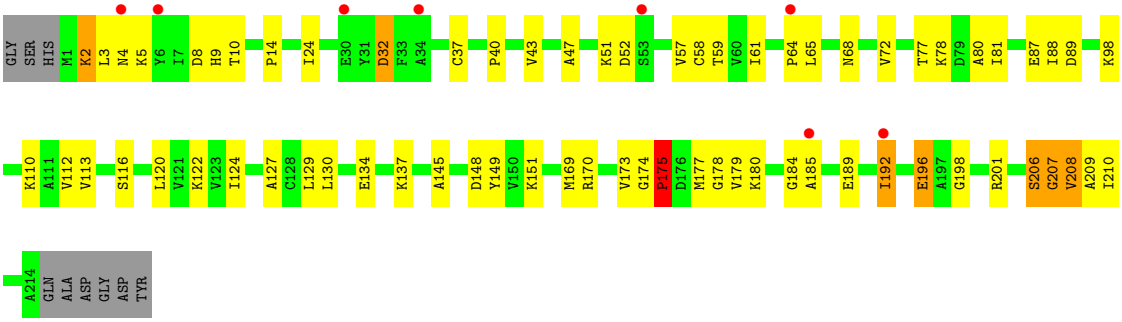
• Molecule 1: Deoxyribose-phosphate aldolase

Chain I:



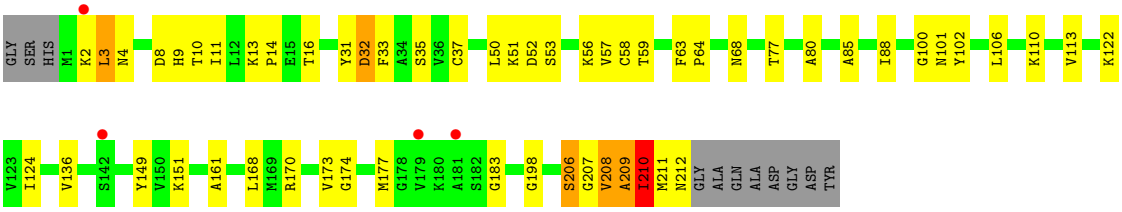
• Molecule 1: Deoxyribose-phosphate aldolase

Chain J:



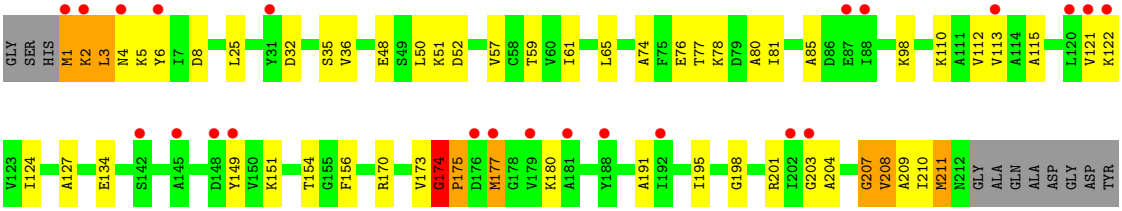
• Molecule 1: Deoxyribose-phosphate aldolase

Chain K:



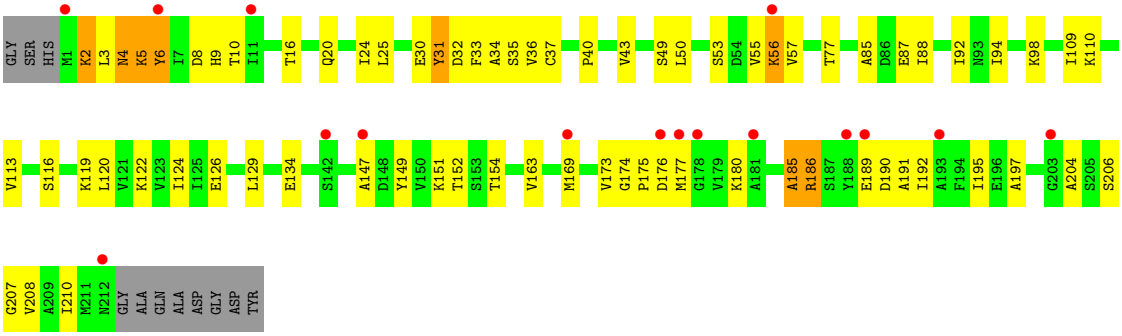
• Molecule 1: Deoxyribose-phosphate aldolase

Chain L:



• Molecule 1: Deoxyribose-phosphate aldolase

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	192.82Å 107.13Å 180.97Å 90.00° 110.50° 90.00°	Depositor
Resolution (Å)	38.31 – 2.80 45.28 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.31-2.80) 99.3 (45.28-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	4.36 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.223 , 0.278 0.234 , 0.282	Depositor DCC
R_{free} test set	4244 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	77.5	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 52.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h+1/2*k-l 0.000 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	20084	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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	0.42	0/1561	0.66	1/2113 (0.0%)
1	B	0.45	0/1553	0.67	2/2103 (0.1%)
1	C	0.41	0/1561	0.63	0/2113
1	D	0.42	0/1569	0.65	2/2124 (0.1%)
1	E	0.47	0/1544	0.69	1/2092 (0.0%)
1	F	0.45	0/1553	0.76	1/2103 (0.0%)
1	G	0.47	0/1553	0.80	3/2103 (0.1%)
1	H	0.49	0/1561	0.68	2/2113 (0.1%)
1	I	0.45	0/1561	0.72	2/2113 (0.1%)
1	J	0.45	0/1578	0.67	2/2136 (0.1%)
1	K	0.46	0/1569	0.70	1/2124 (0.0%)
1	L	0.44	0/1569	0.68	2/2124 (0.1%)
1	M	0.46	0/1569	0.69	2/2124 (0.1%)
All	All	0.45	0/20301	0.69	21/27485 (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	1
1	F	0	3
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
All	All	0	8

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	117	GLY	N-CA-C	-8.09	92.86	113.10
1	G	84	GLY	N-CA-C	-7.70	93.85	113.10
1	B	174	GLY	C-N-CD	6.62	142.30	128.40
1	D	174	GLY	C-N-CD	6.60	142.25	128.40
1	L	174	GLY	C-N-CD	6.54	142.13	128.40
1	J	174	GLY	C-N-CD	6.49	142.03	128.40
1	A	174	GLY	C-N-CD	6.39	141.83	128.40
1	K	174	GLY	C-N-CD	6.21	141.44	128.40
1	E	174	GLY	C-N-CD	6.20	141.43	128.40
1	H	174	GLY	C-N-CD	6.16	141.34	128.40
1	M	174	GLY	C-N-CD	6.12	141.25	128.40
1	G	177	MET	CG-SD-CE	-5.97	90.64	100.20
1	I	174	GLY	C-N-CD	5.90	140.79	128.40
1	H	184	GLY	N-CA-C	-5.75	98.72	113.10
1	D	175	PRO	CA-N-CD	-5.54	103.74	111.50
1	M	185	ALA	C-N-CA	5.44	135.31	121.70
1	G	125	ILE	N-CA-C	-5.37	96.52	111.00
1	J	175	PRO	CA-N-CD	-5.33	104.04	111.50
1	B	1	MET	C-N-CA	5.30	134.94	121.70
1	F	184	GLY	N-CA-C	-5.12	100.30	113.10
1	L	175	PRO	CA-N-CD	-5.03	104.46	111.50

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	185	ALA	Peptide
1	F	148	ASP	Peptide
1	F	185	ALA	Peptide
1	F	86	ASP	Peptide
1	G	143	GLN	Peptide
1	H	185	ALA	Peptide
1	I	117	GLY	Peptide
1	J	2	LYS	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	1544	0	1570	34	0
1	B	1536	0	1561	33	0
1	C	1544	0	1570	41	0
1	D	1552	0	1574	44	0
1	E	1527	0	1545	35	0
1	F	1536	0	1556	84	0
1	G	1536	0	1560	114	0
1	H	1544	0	1570	34	0
1	I	1544	0	1570	54	0
1	J	1561	0	1584	55	0
1	K	1552	0	1576	61	0
1	L	1552	0	1576	73	0
1	M	1552	0	1576	56	0
2	C	3	0	0	0	0
2	D	1	0	0	0	0
All	All	20084	0	20388	701	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 17.

All (701) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1:MET:SD	1:G:3:LEU:HD11	1.65	1.36
1:L:209:ALA:CB	1:L:211:MET:HB3	1.63	1.28
1:G:1:MET:O	1:G:3:LEU:N	1.72	1.20
1:G:144:GLU:OE2	1:G:177:MET:SD	1.98	1.19
1:G:110:LYS:HG2	1:G:145:ALA:HB1	1.25	1.14
1:C:2:LYS:HE3	1:C:3:LEU:H	1.03	1.13
1:D:143:GLN:HB2	1:D:177:MET:HE1	1.32	1.12
1:L:209:ALA:HB2	1:L:211:MET:HB3	1.14	1.10
1:K:207:GLY:HA2	1:K:208:VAL:HG13	1.36	1.06
1:G:110:LYS:CG	1:G:145:ALA:HB1	1.87	1.04
1:F:89:ASP:OD1	1:F:122:LYS:HD2	1.57	1.03
1:G:144:GLU:O	1:G:146:GLY:N	1.81	1.02
1:G:137:LYS:O	1:G:141:LEU:HB2	1.59	1.01
1:G:1:MET:O	1:G:3:LEU:HG	1.60	1.00
1:F:113:VAL:O	1:F:116:SER:HB3	1.60	1.00
1:D:143:GLN:CB	1:D:177:MET:HE1	1.93	0.99
1:L:209:ALA:HB1	1:L:211:MET:N	1.79	0.98
1:K:173:VAL:CG1	1:K:177:MET:HB3	1.94	0.98
1:G:86:ASP:HA	1:G:119:LYS:HD2	1.45	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:LYS:NZ	1:F:32:ASP:OD2	1.97	0.97
1:G:1:MET:SD	1:G:3:LEU:CD1	2.52	0.97
1:L:208:VAL:HG23	1:L:209:ALA:HB2	1.47	0.96
1:L:2:LYS:HE2	1:L:6:TYR:HE1	1.30	0.96
1:G:147:ALA:HB1	1:G:148:ASP:HA	1.47	0.96
1:L:207:GLY:N	1:L:208:VAL:O	1.98	0.96
1:G:56:LYS:HG2	1:G:86:ASP:OD1	1.64	0.95
1:K:208:VAL:O	1:K:210:ILE:N	2.00	0.95
1:K:161:ALA:H	1:K:183:GLY:HA3	1.30	0.94
1:F:199:ALA:HA	1:F:200:SER:HB3	1.48	0.93
1:K:50:LEU:O	1:K:53:SER:OG	1.85	0.92
1:M:185:ALA:HA	1:M:186:ARG:HB2	1.51	0.92
1:F:114:ALA:O	1:F:116:SER:N	2.02	0.92
1:C:2:LYS:HE3	1:C:3:LEU:N	1.85	0.91
1:L:207:GLY:HA2	1:L:210:ILE:CG2	2.00	0.91
1:J:2:LYS:HD2	1:J:3:LEU:H	1.36	0.90
1:L:209:ALA:CB	1:L:211:MET:CB	2.49	0.89
1:G:142:SER:C	1:G:144:GLU:HA	1.91	0.89
1:I:14:PRO:HG3	1:J:65:LEU:HD22	1.54	0.89
1:E:124:ILE:HG12	1:E:151:LYS:HD3	1.53	0.88
1:L:209:ALA:HB1	1:L:211:MET:HB3	1.55	0.88
1:C:2:LYS:CE	1:C:3:LEU:H	1.87	0.88
1:F:179:VAL:HG23	1:F:199:ALA:HB2	1.53	0.87
1:K:14:PRO:HG3	1:L:65:LEU:HD22	1.57	0.87
1:I:87:GLU:OE2	1:I:201:ARG:NH2	2.08	0.86
1:I:87:GLU:CD	1:I:201:ARG:HH22	1.77	0.86
1:L:209:ALA:HA	1:L:210:ILE:C	1.94	0.85
1:C:10:THR:HB	1:C:204:ALA:HB1	1.59	0.85
1:F:117:GLY:HA3	1:F:119:LYS:O	1.77	0.85
1:K:207:GLY:CA	1:K:208:VAL:HG13	2.07	0.85
1:L:2:LYS:HE2	1:L:6:TYR:CE1	2.12	0.85
1:G:117:GLY:HA3	1:G:119:LYS:N	1.92	0.84
1:A:77:THR:HG21	1:A:112:VAL:HG13	1.58	0.84
1:C:56:LYS:NZ	1:I:176:ASP:OD2	2.10	0.84
1:G:109:ILE:HD11	1:G:123:VAL:HG21	1.60	0.84
1:J:169:MET:O	1:J:173:VAL:HG12	1.78	0.83
1:F:179:VAL:O	1:F:199:ALA:HB1	1.78	0.83
1:J:189:GLU:HA	1:J:192:ILE:HG22	1.58	0.83
1:G:144:GLU:OE2	1:G:177:MET:CE	2.27	0.83
1:L:209:ALA:N	1:L:210:ILE:HG22	1.94	0.83
1:L:209:ALA:HA	1:L:210:ILE:CG2	2.09	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:208:VAL:HA	1:J:210:ILE:H	1.42	0.82
1:A:65:LEU:HD22	1:B:14:PRO:HG3	1.62	0.82
1:I:3:LEU:HD12	1:I:3:LEU:O	1.78	0.82
1:L:209:ALA:HB1	1:L:211:MET:CB	2.09	0.82
1:G:113:VAL:HG21	1:G:146:GLY:HA3	1.61	0.82
1:L:207:GLY:HA2	1:L:210:ILE:HG21	1.61	0.81
1:F:152:THR:OG1	1:F:182:SER:O	1.99	0.81
1:G:110:LYS:CG	1:G:145:ALA:CB	2.58	0.81
1:L:209:ALA:CA	1:L:210:ILE:HG22	2.10	0.81
1:G:110:LYS:HG2	1:G:145:ALA:CB	2.08	0.81
1:B:77:THR:HG21	1:B:112:VAL:HG13	1.61	0.81
1:F:199:ALA:HA	1:F:200:SER:CB	2.10	0.81
1:B:3:LEU:HD11	1:B:188:TYR:HE1	1.45	0.81
1:G:143:GLN:N	1:G:144:GLU:HA	1.93	0.80
1:K:124:ILE:HG12	1:K:151:LYS:HD3	1.62	0.80
1:H:124:ILE:HG12	1:H:151:LYS:HD2	1.61	0.80
1:F:11:ILE:HB	1:F:24:ILE:HD12	1.62	0.80
1:F:161:ALA:H	1:F:183:GLY:HA3	1.47	0.80
1:L:173:VAL:HG21	1:L:177:MET:SD	2.22	0.80
1:E:169:MET:O	1:E:173:VAL:HG22	1.83	0.79
1:H:206:SER:O	1:H:209:ALA:N	2.15	0.79
1:M:169:MET:O	1:M:173:VAL:HG12	1.82	0.79
1:L:2:LYS:CE	1:L:6:TYR:HE1	1.95	0.79
1:A:124:ILE:HG12	1:A:151:LYS:HD3	1.65	0.79
1:F:116:SER:OG	1:F:117:GLY:N	2.15	0.79
1:L:209:ALA:HB1	1:L:211:MET:CA	2.13	0.79
1:C:9:HIS:HD2	1:C:24:ILE:HG23	1.48	0.79
1:F:77:THR:HG21	1:F:112:VAL:HG13	1.64	0.78
1:F:170:ARG:NH1	1:F:177:MET:O	2.15	0.78
1:J:77:THR:HG21	1:J:112:VAL:HG13	1.63	0.78
1:G:194:PHE:O	1:G:199:ALA:HB2	1.84	0.78
1:D:143:GLN:CB	1:D:177:MET:CE	2.62	0.77
1:G:5:LYS:H	1:G:5:LYS:HD2	1.50	0.76
1:E:14:PRO:HG3	1:F:65:LEU:HD22	1.64	0.76
1:C:124:ILE:HG12	1:C:151:LYS:HD3	1.67	0.76
1:D:124:ILE:HG12	1:D:151:LYS:HD3	1.66	0.76
1:L:2:LYS:CE	1:L:6:TYR:CE1	2.68	0.76
1:I:90:MET:SD	1:I:112:VAL:HG11	2.25	0.76
1:E:206:SER:O	1:E:208:VAL:N	2.17	0.76
1:F:113:VAL:O	1:F:114:ALA:O	2.04	0.76
1:J:10:THR:HG22	1:J:37:CYS:HB3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:35:SER:HB3	1:M:56:LYS:HE2	1.67	0.75
1:D:143:GLN:HB2	1:D:177:MET:CE	2.15	0.75
1:L:208:VAL:CG2	1:L:209:ALA:HB2	2.17	0.75
1:F:179:VAL:CG2	1:F:199:ALA:HB2	2.16	0.75
1:B:169:MET:O	1:B:173:VAL:HG22	1.86	0.75
1:F:124:ILE:HG12	1:F:151:LYS:HD3	1.70	0.74
1:M:50:LEU:HD12	1:M:57:VAL:HG12	1.69	0.74
1:D:189:GLU:HA	1:D:192:ILE:HG12	1.70	0.73
1:K:173:VAL:HG11	1:K:177:MET:HB3	1.68	0.73
1:M:185:ALA:HB1	1:M:190:ASP:HB3	1.69	0.73
1:H:169:MET:O	1:H:173:VAL:HG22	1.89	0.73
1:L:208:VAL:HG23	1:L:209:ALA:CB	2.17	0.73
1:H:50:LEU:HD12	1:H:57:VAL:HG12	1.71	0.73
1:B:1:MET:N	1:B:2:LYS:HB2	2.03	0.73
1:F:179:VAL:O	1:F:199:ALA:CB	2.37	0.73
1:I:197:ALA:N	1:I:198:GLY:HA2	2.04	0.72
1:K:207:GLY:HA3	1:K:208:VAL:C	2.10	0.72
1:L:209:ALA:CB	1:L:211:MET:N	2.53	0.72
1:I:87:GLU:OE1	1:I:201:ARG:NH1	2.23	0.72
1:G:1:MET:C	1:G:3:LEU:H	1.91	0.72
1:B:40:PRO:O	1:B:43:VAL:HG12	1.90	0.71
1:G:140:GLN:O	1:G:143:GLN:HB2	1.91	0.71
1:J:2:LYS:HD2	1:J:3:LEU:N	2.04	0.71
1:L:209:ALA:HA	1:L:210:ILE:HG22	1.70	0.71
1:G:86:ASP:CA	1:G:119:LYS:HD2	2.21	0.71
1:C:2:LYS:HE3	1:C:3:LEU:HB2	1.73	0.71
1:J:124:ILE:HG12	1:J:151:LYS:HD3	1.73	0.70
1:E:208:VAL:HG13	1:E:210:ILE:HG22	1.72	0.70
1:J:206:SER:O	1:J:208:VAL:N	2.24	0.70
1:K:173:VAL:HG12	1:K:177:MET:HB3	1.73	0.70
1:D:173:VAL:HG21	1:D:177:MET:SD	2.32	0.70
1:J:170:ARG:HH11	1:J:179:VAL:HG13	1.55	0.70
1:G:124:ILE:HG12	1:G:151:LYS:HD3	1.73	0.70
1:B:3:LEU:HD11	1:B:188:TYR:CE1	2.25	0.69
1:G:147:ALA:HB3	1:G:148:ASP:CG	2.12	0.69
1:I:124:ILE:HG12	1:I:151:LYS:HD3	1.75	0.69
1:B:184:GLY:H	1:B:185:ALA:HB2	1.58	0.69
1:L:77:THR:HG21	1:L:112:VAL:HG13	1.74	0.69
1:G:117:GLY:CA	1:G:118:ASP:HB2	2.23	0.69
1:M:173:VAL:HG21	1:M:177:MET:HB3	1.75	0.69
1:F:77:THR:HG21	1:F:112:VAL:CG1	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:147:ALA:CB	1:G:148:ASP:HA	2.22	0.69
1:I:192:ILE:O	1:I:196:GLU:HG3	1.92	0.68
1:G:173:VAL:HG11	1:G:177:MET:SD	2.33	0.68
1:M:77:THR:HG23	1:M:88:ILE:HG13	1.75	0.68
1:A:169:MET:O	1:A:173:VAL:HG12	1.94	0.68
1:K:207:GLY:HA2	1:K:208:VAL:CG1	2.20	0.68
1:G:110:LYS:HG3	1:G:145:ALA:CB	2.23	0.68
1:K:206:SER:HB3	1:K:208:VAL:HG22	1.76	0.67
1:C:90:MET:SD	1:C:112:VAL:HG11	2.34	0.67
1:H:101:ASN:OD1	1:H:104:LEU:HB2	1.94	0.67
1:K:35:SER:HB3	1:K:56:LYS:HB2	1.76	0.67
1:E:203:GLY:O	1:E:204:ALA:HB2	1.93	0.67
1:I:176:ASP:OD1	1:I:176:ASP:N	2.26	0.67
1:G:1:MET:C	1:G:3:LEU:N	2.46	0.67
1:L:50:LEU:HD12	1:L:57:VAL:HG12	1.76	0.66
1:J:196:GLU:O	1:J:196:GLU:HG2	1.95	0.66
1:G:2:LYS:O	1:G:4:ASN:CG	2.34	0.66
1:E:113:VAL:O	1:E:116:SER:HB3	1.95	0.66
1:J:4:ASN:ND2	1:J:32:ASP:O	2.28	0.66
1:L:113:VAL:HG12	1:L:121:VAL:HG21	1.78	0.66
1:A:40:PRO:O	1:A:43:VAL:HG12	1.96	0.66
1:F:10:THR:HG22	1:F:37:CYS:HB2	1.78	0.66
1:F:196:GLU:O	1:F:196:GLU:HG3	1.97	0.65
1:G:47:ALA:HB3	1:G:83:ASN:OD1	1.96	0.65
1:F:200:SER:O	1:F:201:ARG:HB2	1.96	0.65
1:M:207:GLY:HA3	1:M:208:VAL:HB	1.78	0.64
1:C:9:HIS:CD2	1:C:24:ILE:HG23	2.31	0.64
1:A:87:GLU:HG2	1:A:120:LEU:HB3	1.80	0.64
1:C:57:VAL:HG23	1:C:85:ALA:HA	1.80	0.64
1:E:173:VAL:HG11	1:E:177:MET:HE2	1.77	0.64
1:F:5:LYS:NZ	1:F:32:ASP:O	2.30	0.64
1:B:61:ILE:HG13	1:B:77:THR:HG22	1.80	0.64
1:K:110:LYS:HA	1:K:113:VAL:HG12	1.80	0.64
1:L:61:ILE:HG13	1:L:77:THR:HG22	1.79	0.64
1:G:31:TYR:O	1:G:33:PHE:N	2.31	0.63
1:K:2:LYS:HB3	1:K:3:LEU:HA	1.79	0.63
1:D:143:GLN:HG3	1:D:177:MET:HE3	1.79	0.63
1:G:144:GLU:C	1:G:146:GLY:N	2.50	0.63
1:E:206:SER:C	1:E:208:VAL:H	2.01	0.63
1:G:206:SER:O	1:G:208:VAL:N	2.31	0.63
1:L:173:VAL:CG2	1:L:177:MET:SD	2.86	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:209:ALA:CA	1:L:210:ILE:C	2.66	0.63
1:J:9:HIS:CD2	1:J:24:ILE:HG23	2.33	0.63
1:M:189:GLU:HA	1:M:192:ILE:HG12	1.80	0.63
1:G:2:LYS:HD3	1:G:4:ASN:ND2	2.13	0.63
1:I:8:ASP:OD1	1:I:35:SER:OG	2.17	0.63
1:G:126:GLU:HG3	1:G:153:SER:HA	1.80	0.62
1:D:143:GLN:CA	1:D:177:MET:HE1	2.28	0.62
1:G:78:LYS:C	1:G:80:ALA:H	2.01	0.62
1:K:10:THR:HG22	1:K:37:CYS:HB3	1.80	0.62
1:A:185:ALA:HB2	1:A:194:PHE:HE2	1.64	0.62
1:H:207:GLY:O	1:H:208:VAL:HG22	2.00	0.62
1:F:195:ILE:HA	1:F:199:ALA:O	2.00	0.62
1:G:195:ILE:HA	1:G:199:ALA:HB3	1.80	0.62
1:M:98:LYS:NZ	1:M:134:GLU:OE1	2.32	0.62
1:H:207:GLY:O	1:H:208:VAL:HG13	2.00	0.62
1:F:199:ALA:CA	1:F:200:SER:HB3	2.25	0.62
1:G:1:MET:O	1:G:2:LYS:C	2.38	0.61
1:L:1:MET:C	1:L:2:LYS:HG3	2.21	0.61
1:M:87:GLU:HG2	1:M:120:LEU:HB3	1.80	0.61
1:F:9:HIS:HD2	1:F:24:ILE:HG23	1.64	0.61
1:J:170:ARG:HH12	1:J:178:GLY:HA2	1.65	0.61
1:L:208:VAL:O	1:L:208:VAL:HG13	2.01	0.61
1:G:109:ILE:HG23	1:G:145:ALA:HB3	1.82	0.61
1:K:4:ASN:HB3	1:K:210:ILE:HD11	1.83	0.61
1:J:208:VAL:N	1:J:209:ALA:HB3	2.15	0.61
1:L:1:MET:O	1:L:2:LYS:HG3	2.00	0.60
1:M:3:LEU:O	1:M:5:LYS:N	2.34	0.60
1:L:124:ILE:HG12	1:L:151:LYS:HD3	1.82	0.60
1:F:37:CYS:HA	1:F:58:CYS:O	2.01	0.60
1:G:117:GLY:HA3	1:G:119:LYS:H	1.65	0.60
1:K:11:ILE:HG12	1:K:16:THR:HG21	1.83	0.60
1:J:173:VAL:HG22	1:J:173:VAL:O	2.02	0.60
1:J:206:SER:C	1:J:208:VAL:H	2.06	0.60
1:M:173:VAL:CG2	1:M:177:MET:HB3	2.32	0.60
1:D:173:VAL:HG22	1:D:173:VAL:O	2.02	0.59
1:G:5:LYS:HD2	1:G:5:LYS:N	2.14	0.59
1:H:208:VAL:C	1:H:210:ILE:H	2.06	0.59
1:H:186:ARG:HA	1:H:206:SER:OG	2.02	0.59
1:H:192:ILE:O	1:H:196:GLU:HG2	2.01	0.59
1:I:197:ALA:N	1:I:198:GLY:CA	2.66	0.59
1:B:1:MET:H2	1:B:2:LYS:HB2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:86:ASP:HA	1:I:119:LYS:HD3	1.84	0.59
1:B:124:ILE:HG12	1:B:151:LYS:HD3	1.84	0.59
1:F:9:HIS:CD2	1:F:24:ILE:HG23	2.37	0.59
1:D:143:GLN:HG3	1:D:177:MET:CE	2.31	0.59
1:M:185:ALA:CA	1:M:186:ARG:HB2	2.30	0.59
1:E:173:VAL:CG1	1:E:177:MET:HE2	2.32	0.59
1:G:1:MET:O	1:G:3:LEU:CG	2.45	0.59
1:G:57:VAL:HG23	1:G:85:ALA:HA	1.84	0.59
1:G:117:GLY:HA2	1:G:118:ASP:HB2	1.83	0.58
1:I:175:PRO:HG2	1:I:176:ASP:OD1	2.03	0.58
1:I:98:LYS:NZ	1:I:134:GLU:OE1	2.37	0.58
1:B:113:VAL:O	1:B:116:SER:HB3	2.02	0.58
1:D:143:GLN:CG	1:D:177:MET:CE	2.82	0.58
1:H:104:LEU:O	1:H:104:LEU:HD23	2.03	0.58
1:C:208:VAL:HG23	1:C:208:VAL:O	2.03	0.58
1:F:87:GLU:OE2	1:F:122:LYS:CE	2.51	0.58
1:G:144:GLU:OE2	1:G:177:MET:HE1	2.03	0.58
1:K:77:THR:HG23	1:K:88:ILE:HG13	1.85	0.58
1:L:208:VAL:HA	1:L:209:ALA:HB2	1.85	0.58
1:G:147:ALA:HB1	1:G:148:ASP:CA	2.30	0.58
1:L:209:ALA:HB2	1:L:211:MET:CB	2.08	0.58
1:A:209:ALA:C	1:A:211:MET:H	2.07	0.58
1:M:163:VAL:HG13	1:M:197:ALA:HB2	1.86	0.58
1:B:151:LYS:HE3	1:B:180:LYS:HE2	1.86	0.57
1:F:2:LYS:HD3	1:F:2:LYS:N	2.19	0.57
1:I:170:ARG:NH2	1:I:177:MET:O	2.37	0.57
1:J:170:ARG:HD3	1:J:198:GLY:O	2.02	0.57
1:J:148:ASP:O	1:J:149:TYR:HD1	1.87	0.57
1:E:168:LEU:O	1:E:172:THR:HG23	2.04	0.57
1:M:4:ASN:O	1:M:33:PHE:HA	2.04	0.57
1:F:61:ILE:HG13	1:F:77:THR:HG22	1.87	0.57
1:L:25:LEU:HD23	1:L:36:VAL:HG21	1.87	0.57
1:M:175:PRO:O	1:M:176:ASP:HB2	2.05	0.56
1:G:198:GLY:O	1:G:199:ALA:HB2	2.04	0.56
1:D:143:GLN:HA	1:D:177:MET:CE	2.34	0.56
1:G:95:GLY:O	1:G:99:THR:HG23	2.06	0.56
1:G:101:ASN:O	1:G:102:TYR:HB2	2.05	0.56
1:G:2:LYS:O	1:G:4:ASN:OD1	2.22	0.56
1:K:8:ASP:OD2	1:K:122:LYS:NZ	2.39	0.56
1:D:173:VAL:CG2	1:D:177:MET:SD	2.94	0.56
1:C:8:ASP:OD1	1:C:35:SER:OG	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:10:THR:HG23	1:M:37:CYS:HB3	1.88	0.56
1:C:143:GLN:HG3	1:C:177:MET:HE3	1.87	0.55
1:G:147:ALA:HB3	1:G:148:ASP:OD1	2.06	0.55
1:I:173:VAL:CG2	1:I:177:MET:SD	2.94	0.55
1:L:4:ASN:HB3	1:L:210:ILE:HD11	1.87	0.55
1:B:3:LEU:HD12	1:B:3:LEU:H	1.71	0.55
1:F:9:HIS:NE2	1:F:27:GLU:OE2	2.29	0.55
1:J:98:LYS:HE3	1:J:129:LEU:O	2.06	0.55
1:L:151:LYS:HE3	1:L:180:LYS:HE2	1.88	0.55
1:A:185:ALA:HB2	1:A:194:PHE:CE2	2.42	0.55
1:G:57:VAL:HG23	1:G:57:VAL:O	2.06	0.55
1:G:147:ALA:CB	1:G:148:ASP:CA	2.84	0.55
1:K:51:LYS:O	1:K:52:ASP:HB2	2.07	0.55
1:L:209:ALA:HB1	1:L:211:MET:H	1.65	0.55
1:C:40:PRO:HA	1:C:43:VAL:HG23	1.89	0.55
1:D:143:GLN:CG	1:D:177:MET:HE3	2.37	0.55
1:G:1:MET:HB2	1:G:3:LEU:HG	1.88	0.55
1:I:4:ASN:ND2	1:I:32:ASP:O	2.40	0.55
1:J:78:LYS:NZ	1:J:81:ILE:HD11	2.21	0.55
1:F:87:GLU:OE2	1:F:122:LYS:NZ	2.38	0.55
1:G:60:VAL:HG21	1:G:63:PHE:CD1	2.42	0.55
1:D:11:ILE:HG13	1:D:16:THR:HG21	1.89	0.55
1:K:207:GLY:C	1:K:208:VAL:HG13	2.26	0.55
1:L:203:GLY:O	1:L:204:ALA:HB2	2.07	0.55
1:J:5:LYS:NZ	1:J:32:ASP:OD1	2.40	0.55
1:F:130:LEU:HB3	1:F:134:GLU:HB2	1.89	0.54
1:G:6:TYR:CE1	1:G:199:ALA:O	2.61	0.54
1:J:113:VAL:O	1:J:116:SER:HB3	2.07	0.54
1:F:113:VAL:C	1:F:116:SER:HB3	2.26	0.54
1:H:40:PRO:O	1:H:43:VAL:HG22	2.07	0.54
1:D:4:ASN:ND2	1:D:32:ASP:O	2.40	0.54
1:F:23:LYS:O	1:F:27:GLU:HG3	2.06	0.54
1:F:117:GLY:CA	1:F:118:ASP:CB	2.85	0.54
1:C:149:TYR:OH	1:C:200:SER:OG	2.12	0.54
1:F:87:GLU:OE2	1:F:201:ARG:NH2	2.40	0.54
1:K:173:VAL:CG1	1:K:177:MET:SD	2.95	0.54
1:F:121:VAL:HG23	1:F:121:VAL:O	2.07	0.54
1:G:144:GLU:C	1:G:146:GLY:H	2.03	0.54
1:H:185:ALA:HB3	1:H:190:ASP:HB3	1.88	0.54
1:I:3:LEU:HD12	1:I:3:LEU:C	2.24	0.54
1:E:173:VAL:HG11	1:E:177:MET:CE	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:110:LYS:HG3	1:G:145:ALA:HB1	1.79	0.54
1:A:173:VAL:HG22	1:A:177:MET:HB3	1.90	0.54
1:G:195:ILE:HA	1:G:199:ALA:CB	2.38	0.54
1:A:113:VAL:O	1:A:116:SER:HB3	2.08	0.53
1:F:169:MET:O	1:F:173:VAL:HG12	2.07	0.53
1:A:78:LYS:HG3	1:A:115:ALA:HB1	1.90	0.53
1:M:186:ARG:HA	1:M:206:SER:HB2	1.89	0.53
1:K:161:ALA:N	1:K:183:GLY:HA3	2.13	0.53
1:L:208:VAL:CA	1:L:209:ALA:HB2	2.39	0.53
1:D:8:ASP:OD2	1:D:122:LYS:NZ	2.41	0.53
1:G:34:ALA:O	1:G:55:VAL:O	2.27	0.53
1:M:53:SER:HB3	1:M:55:VAL:HG12	1.89	0.53
1:D:106:LEU:HD23	1:D:110:LYS:NZ	2.24	0.53
1:L:209:ALA:CA	1:L:211:MET:N	2.72	0.53
1:H:203:GLY:O	1:H:204:ALA:HB2	2.09	0.52
1:J:148:ASP:O	1:J:177:MET:HB2	2.09	0.52
1:B:170:ARG:NH1	1:B:177:MET:O	2.42	0.52
1:K:2:LYS:HB2	1:K:3:LEU:HB3	1.89	0.52
1:B:18:GLN:NE2	1:B:22:GLU:OE2	2.37	0.52
1:C:5:LYS:NZ	1:C:32:ASP:OD2	2.42	0.52
1:F:118:ASP:C	1:F:119:LYS:HG3	2.27	0.52
1:K:106:LEU:HG	1:K:110:LYS:HE2	1.91	0.52
1:K:208:VAL:HG23	1:K:209:ALA:N	2.25	0.52
1:G:137:LYS:O	1:G:141:LEU:CB	2.47	0.52
1:I:73:LYS:NZ	1:I:108:ASP:OD2	2.28	0.52
1:K:208:VAL:CG2	1:K:209:ALA:N	2.73	0.52
1:F:120:LEU:HD22	1:F:121:VAL:N	2.24	0.52
1:C:56:LYS:CE	1:I:176:ASP:OD2	2.58	0.52
1:G:206:SER:C	1:G:208:VAL:H	2.14	0.52
1:H:58:CYS:SG	1:H:122:LYS:NZ	2.82	0.52
1:L:98:LYS:NZ	1:L:134:GLU:OE1	2.43	0.52
1:H:87:GLU:HG2	1:H:120:LEU:HB3	1.92	0.51
1:L:208:VAL:C	1:L:210:ILE:HG22	2.31	0.51
1:C:10:THR:CB	1:C:204:ALA:HB1	2.35	0.51
1:K:206:SER:HB3	1:K:208:VAL:CG2	2.40	0.51
1:L:208:VAL:CG2	1:L:209:ALA:CB	2.85	0.51
1:F:177:MET:HG2	1:F:178:GLY:N	2.26	0.51
1:G:2:LYS:HD3	1:G:4:ASN:HD21	1.75	0.51
1:B:130:LEU:HB3	1:B:134:GLU:HB2	1.92	0.51
1:E:40:PRO:HA	1:E:43:VAL:HG23	1.93	0.51
1:F:149:TYR:HB2	1:F:178:GLY:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:44:ALA:HA	1:G:83:ASN:HB3	1.92	0.51
1:L:57:VAL:HG23	1:L:85:ALA:HA	1.92	0.51
1:M:25:LEU:HD23	1:M:36:VAL:HG11	1.93	0.51
1:E:130:LEU:HB3	1:E:134:GLU:HB2	1.92	0.51
1:F:87:GLU:HG2	1:F:122:LYS:HE3	1.92	0.51
1:G:110:LYS:HG3	1:G:145:ALA:HB2	1.90	0.51
1:I:136:VAL:O	1:I:140:GLN:HG3	2.10	0.51
1:K:173:VAL:HG11	1:K:177:MET:SD	2.51	0.51
1:A:8:ASP:OD1	1:A:35:SER:OG	2.27	0.51
1:E:173:VAL:CG1	1:E:177:MET:CE	2.88	0.51
1:G:67:ALA:O	1:H:41:THR:HG23	2.11	0.51
1:K:13:LYS:O	1:K:16:THR:HG23	2.10	0.51
1:D:9:HIS:CD2	1:D:24:ILE:HG23	2.46	0.51
1:H:18:GLN:NE2	1:H:22:GLU:OE2	2.34	0.50
1:M:8:ASP:OD1	1:M:35:SER:OG	2.30	0.50
1:M:110:LYS:HA	1:M:113:VAL:HG22	1.93	0.50
1:F:112:VAL:O	1:F:116:SER:HB2	2.10	0.50
1:F:149:TYR:HE1	1:F:180:LYS:HB2	1.75	0.50
1:I:175:PRO:HD2	1:I:176:ASP:OD1	2.12	0.50
1:J:2:LYS:CD	1:J:3:LEU:H	2.14	0.50
1:F:87:GLU:HG3	1:F:120:LEU:HD13	1.92	0.50
1:G:63:PHE:CE1	1:G:154:THR:HB	2.47	0.50
1:I:173:VAL:HG21	1:I:177:MET:SD	2.51	0.50
1:A:61:ILE:HG13	1:A:77:THR:HG22	1.93	0.50
1:F:117:GLY:HA2	1:F:118:ASP:CB	2.41	0.50
1:B:184:GLY:N	1:B:185:ALA:HB2	2.25	0.50
1:C:48:GLU:O	1:C:48:GLU:HG3	2.10	0.50
1:C:76:GLU:HG3	1:D:72:VAL:HG21	1.93	0.50
1:I:210:ILE:O	1:I:210:ILE:HG22	2.11	0.50
1:K:208:VAL:HG23	1:K:209:ALA:H	1.76	0.50
1:F:120:LEU:CD2	1:F:121:VAL:N	2.75	0.50
1:I:76:GLU:OE1	1:J:68:ASN:ND2	2.39	0.50
1:K:207:GLY:HA3	1:K:208:VAL:O	2.11	0.50
1:A:189:GLU:OE1	1:A:189:GLU:N	2.40	0.50
1:J:61:ILE:HG13	1:J:88:ILE:HG23	1.94	0.49
1:C:2:LYS:CE	1:C:3:LEU:HB2	2.41	0.49
1:J:189:GLU:OE1	1:J:189:GLU:N	2.39	0.49
1:K:173:VAL:HG13	1:K:177:MET:SD	2.52	0.49
1:L:207:GLY:HA2	1:L:210:ILE:HG22	1.90	0.49
1:B:61:ILE:HD12	1:B:76:GLU:HG2	1.95	0.49
1:C:152:THR:HG22	1:C:169:MET:SD	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7:ILE:HB	1:G:33:PHE:CD1	2.48	0.49
1:L:209:ALA:CA	1:L:210:ILE:CG2	2.77	0.49
1:G:44:ALA:HA	1:G:83:ASN:O	2.12	0.49
1:D:143:GLN:CA	1:D:177:MET:CE	2.91	0.49
1:E:64:PRO:HD2	1:F:64:PRO:HD2	1.94	0.49
1:K:122:LYS:HG2	1:K:149:TYR:HB2	1.94	0.49
1:D:106:LEU:HD23	1:D:110:LYS:HZ3	1.76	0.49
1:I:28:ALA:HB1	1:I:55:VAL:HG11	1.95	0.49
1:J:207:GLY:O	1:J:208:VAL:CG1	2.61	0.49
1:G:183:GLY:O	1:G:185:ALA:N	2.43	0.49
1:I:122:LYS:HG2	1:I:149:TYR:HB2	1.94	0.49
1:K:33:PHE:HE1	1:K:210:ILE:HD12	1.76	0.49
1:G:140:GLN:O	1:G:143:GLN:CB	2.58	0.48
1:J:208:VAL:HG23	1:J:208:VAL:O	2.13	0.48
1:I:73:LYS:HD2	1:I:108:ASP:OD1	2.12	0.48
1:M:8:ASP:OD2	1:M:122:LYS:NZ	2.45	0.48
1:G:87:GLU:OE1	1:G:201:ARG:NH1	2.32	0.48
1:G:117:GLY:CA	1:G:119:LYS:H	2.25	0.48
1:J:59:THR:HG21	1:J:80:ALA:HB1	1.96	0.48
1:M:152:THR:HG22	1:M:169:MET:SD	2.53	0.48
1:D:25:LEU:HD23	1:D:36:VAL:HG11	1.95	0.48
1:J:8:ASP:O	1:J:10:THR:HG23	2.13	0.48
1:A:189:GLU:HA	1:A:192:ILE:HG12	1.94	0.48
1:G:101:ASN:C	1:G:103:ASP:H	2.17	0.48
1:J:206:SER:C	1:J:208:VAL:N	2.66	0.48
1:D:210:ILE:O	1:D:210:ILE:HG22	2.13	0.48
1:L:173:VAL:O	1:L:174:GLY:O	2.32	0.48
1:M:124:ILE:HG12	1:M:151:LYS:HD3	1.95	0.48
1:A:23:LYS:O	1:A:27:GLU:HG3	2.13	0.48
1:D:77:THR:HG23	1:D:88:ILE:HG13	1.95	0.48
1:J:173:VAL:HG22	1:J:177:MET:CG	2.43	0.48
1:K:100:GLY:O	1:K:102:TYR:N	2.41	0.48
1:M:3:LEU:O	1:M:6:TYR:N	2.30	0.48
1:M:6:TYR:CE2	1:M:195:ILE:HD13	2.48	0.48
1:M:126:GLU:OE2	1:M:154:THR:OG1	2.27	0.48
1:D:130:LEU:HB3	1:D:134:GLU:HB2	1.94	0.48
1:G:117:GLY:CA	1:G:118:ASP:CB	2.86	0.48
1:K:57:VAL:HG13	1:K:85:ALA:HA	1.96	0.48
1:B:209:ALA:N	1:B:210:ILE:HA	2.28	0.47
1:F:195:ILE:HD12	1:F:196:GLU:N	2.29	0.47
1:I:29:LYS:HE2	1:I:49:SER:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:65:LEU:HD22	1:J:14:PRO:HD3	1.96	0.47
1:K:210:ILE:O	1:K:210:ILE:HG23	2.14	0.47
1:G:64:PRO:HD2	1:H:64:PRO:HD2	1.96	0.47
1:G:70:PRO:HB3	1:G:108:ASP:HA	1.95	0.47
1:G:78:LYS:C	1:G:80:ALA:N	2.68	0.47
1:M:94:ILE:HD13	1:M:129:LEU:HD12	1.96	0.47
1:M:122:LYS:HG2	1:M:149:TYR:HB2	1.96	0.47
1:C:209:ALA:C	1:C:211:MET:H	2.17	0.47
1:H:208:VAL:C	1:H:210:ILE:N	2.68	0.47
1:M:191:ALA:O	1:M:195:ILE:HG13	2.13	0.47
1:I:64:PRO:HD2	1:J:64:PRO:HD2	1.97	0.47
1:B:176:ASP:OD1	1:B:176:ASP:N	2.44	0.47
1:E:136:VAL:O	1:E:140:GLN:HG3	2.14	0.47
1:I:209:ALA:C	1:I:211:MET:H	2.18	0.47
1:J:10:THR:HG22	1:J:37:CYS:CB	2.43	0.47
1:M:116:SER:OG	1:M:119:LYS:O	2.31	0.47
1:A:9:HIS:HD2	1:A:24:ILE:HG23	1.79	0.47
1:F:151:LYS:CG	1:F:182:SER:HB2	2.45	0.47
1:K:212:ASN:OD1	1:K:212:ASN:N	2.47	0.47
1:C:151:LYS:HE3	1:C:180:LYS:HE2	1.97	0.47
1:K:209:ALA:C	1:K:211:MET:H	2.17	0.47
1:E:206:SER:C	1:E:208:VAL:N	2.65	0.47
1:J:173:VAL:CG2	1:J:177:MET:CG	2.93	0.47
1:K:51:LYS:O	1:K:51:LYS:HG3	2.14	0.47
1:L:77:THR:O	1:L:81:ILE:HG23	2.15	0.47
1:D:143:GLN:HA	1:D:177:MET:HE2	1.96	0.47
1:H:61:ILE:HD12	1:H:76:GLU:HG2	1.96	0.47
1:J:122:LYS:HG2	1:J:149:TYR:HB2	1.97	0.47
1:M:152:THR:HG23	1:M:180:LYS:O	2.15	0.47
1:F:117:GLY:HA2	1:F:118:ASP:HB3	1.96	0.46
1:B:1:MET:H3	1:B:2:LYS:HB2	1.80	0.46
1:G:96:ALA:O	1:G:100:GLY:HA2	2.16	0.46
1:J:37:CYS:HA	1:J:58:CYS:O	2.16	0.46
1:K:2:LYS:HB3	1:K:3:LEU:CA	2.44	0.46
1:M:40:PRO:HA	1:M:43:VAL:HG23	1.97	0.46
1:B:9:HIS:CD2	1:B:24:ILE:HG23	2.50	0.46
1:D:40:PRO:HA	1:D:43:VAL:HG23	1.96	0.46
1:G:168:LEU:O	1:G:172:THR:HG23	2.16	0.46
1:G:206:SER:C	1:G:208:VAL:N	2.69	0.46
1:J:78:LYS:HD3	1:J:81:ILE:HD11	1.97	0.46
1:J:208:VAL:HA	1:J:210:ILE:N	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:208:VAL:N	1:E:209:ALA:HB3	2.30	0.46
1:F:50:LEU:HD23	1:F:50:LEU:HA	1.78	0.46
1:I:86:ASP:O	1:I:119:LYS:HB3	2.16	0.46
1:M:57:VAL:HG23	1:M:85:ALA:HA	1.97	0.46
1:E:150:VAL:HG13	1:E:177:MET:HE3	1.98	0.46
1:M:35:SER:HB3	1:M:56:LYS:CE	2.42	0.46
1:D:143:GLN:HA	1:D:177:MET:HE1	1.96	0.46
1:F:118:ASP:O	1:F:119:LYS:HD2	2.16	0.46
1:G:192:ILE:HA	1:G:195:ILE:HB	1.98	0.46
1:H:4:ASN:ND2	1:H:32:ASP:O	2.49	0.46
1:I:116:SER:OG	1:I:118:ASP:HA	2.16	0.46
1:K:31:TYR:CD2	1:K:210:ILE:HG21	2.51	0.46
1:C:9:HIS:CD2	1:C:24:ILE:HD12	2.50	0.46
1:C:204:ALA:O	1:C:205:SER:O	2.33	0.46
1:F:152:THR:HG22	1:F:169:MET:SD	2.56	0.46
1:G:40:PRO:O	1:G:43:VAL:HG22	2.16	0.46
1:C:2:LYS:HG3	1:C:3:LEU:N	2.31	0.46
1:I:40:PRO:HA	1:I:43:VAL:HG23	1.98	0.46
1:E:122:LYS:HG2	1:E:149:TYR:HB2	1.96	0.45
1:F:120:LEU:HD22	1:F:120:LEU:C	2.36	0.45
1:G:55:VAL:O	1:G:56:LYS:HB2	2.15	0.45
1:E:124:ILE:CG1	1:E:151:LYS:HD3	2.35	0.45
1:F:22:GLU:HA	1:F:25:LEU:HD12	1.98	0.45
1:F:66:GLY:O	1:F:93:ASN:HA	2.16	0.45
1:G:51:LYS:HG3	1:G:52:ASP:H	1.81	0.45
1:L:3:LEU:O	1:L:4:ASN:C	2.52	0.45
1:C:207:GLY:C	1:C:209:ALA:H	2.20	0.45
1:I:56:LYS:HG2	1:I:86:ASP:OD2	2.16	0.45
1:I:152:THR:HG22	1:I:169:MET:SD	2.56	0.45
1:J:130:LEU:HB3	1:J:134:GLU:HB2	1.99	0.45
1:L:207:GLY:CA	1:L:208:VAL:C	2.84	0.45
1:H:1:MET:HG2	1:H:2:LYS:H	1.81	0.45
1:I:148:ASP:O	1:I:149:TYR:HD1	1.99	0.45
1:J:89:ASP:OD1	1:J:122:LYS:HD2	2.16	0.45
1:A:122:LYS:HG2	1:A:149:TYR:HB2	1.99	0.45
1:E:132:ASP:HA	1:E:135:LYS:HD2	1.98	0.45
1:J:47:ALA:HA	1:J:57:VAL:HG21	1.98	0.45
1:A:9:HIS:CD2	1:A:24:ILE:HG23	2.52	0.45
1:D:122:LYS:HG2	1:D:149:TYR:HB2	1.98	0.45
1:G:109:ILE:HG23	1:G:145:ALA:CB	2.46	0.45
1:G:143:GLN:N	1:G:144:GLU:CA	2.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:11:ILE:CG2	1:H:24:ILE:HD12	2.47	0.45
1:I:77:THR:OG1	1:I:112:VAL:HG23	2.17	0.45
1:M:185:ALA:CB	1:M:190:ASP:HB3	2.43	0.45
1:D:151:LYS:HE3	1:D:180:LYS:HE2	1.98	0.45
1:G:102:TYR:HA	1:G:141:LEU:HD11	1.99	0.45
1:K:207:GLY:CA	1:K:208:VAL:CG1	2.85	0.45
1:E:152:THR:HG22	1:E:169:MET:SD	2.57	0.45
1:F:120:LEU:CD2	1:F:120:LEU:C	2.85	0.45
1:A:173:VAL:HG21	1:A:177:MET:SD	2.57	0.45
1:H:51:LYS:O	1:H:52:ASP:HB2	2.16	0.45
1:J:87:GLU:OE2	1:J:201:ARG:NH1	2.46	0.45
1:K:68:ASN:ND2	1:L:76:GLU:OE2	2.50	0.45
1:M:151:LYS:HE3	1:M:180:LYS:HE2	1.98	0.45
1:D:9:HIS:HD2	1:D:24:ILE:HG23	1.82	0.44
1:D:206:SER:HB3	1:D:208:VAL:HG22	1.99	0.44
1:F:136:VAL:O	1:F:140:GLN:HG3	2.17	0.44
1:B:184:GLY:HA3	1:B:194:PHE:CE2	2.52	0.44
1:F:195:ILE:C	1:F:197:ALA:H	2.21	0.44
1:K:136:VAL:HG22	1:K:168:LEU:HD21	1.99	0.44
1:A:4:ASN:C	1:A:6:TYR:H	2.19	0.44
1:A:61:ILE:HG13	1:A:88:ILE:HG23	1.98	0.44
1:B:147:ALA:O	1:B:177:MET:HE3	2.17	0.44
1:E:25:LEU:HD23	1:E:36:VAL:HG21	1.98	0.44
1:F:148:ASP:O	1:F:149:TYR:HB3	2.17	0.44
1:L:59:THR:HG21	1:L:80:ALA:HB1	1.99	0.44
1:C:2:LYS:HE3	1:C:3:LEU:CB	2.46	0.44
1:C:48:GLU:HG3	1:C:51:LYS:NZ	2.33	0.44
1:L:51:LYS:O	1:L:52:ASP:HB2	2.17	0.44
1:D:61:ILE:HG13	1:D:88:ILE:HG23	2.00	0.44
1:K:170:ARG:NH2	1:K:198:GLY:O	2.39	0.44
1:A:2:LYS:HB3	1:A:6:TYR:CE1	2.53	0.44
1:H:130:LEU:HB3	1:H:134:GLU:HB2	2.00	0.44
1:I:76:GLU:HG3	1:J:72:VAL:HG21	1.98	0.44
1:J:110:LYS:HE2	1:J:145:ALA:HA	2.00	0.44
1:D:8:ASP:OD1	1:D:35:SER:OG	2.34	0.44
1:F:151:LYS:CE	1:F:182:SER:OG	2.66	0.44
1:G:93:ASN:HD22	1:G:96:ALA:CB	2.29	0.44
1:G:122:LYS:HA	1:G:149:TYR:HB2	1.99	0.44
1:H:57:VAL:HG23	1:H:85:ALA:HA	2.00	0.44
1:A:173:VAL:HG22	1:A:173:VAL:O	2.18	0.44
1:G:120:LEU:HD21	1:G:149:TYR:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:104:LEU:C	1:H:104:LEU:CD2	2.86	0.44
1:I:12:LEU:HD13	1:I:63:PHE:CE2	2.53	0.44
1:I:57:VAL:HG13	1:I:85:ALA:HA	2.00	0.44
1:K:173:VAL:HG12	1:K:173:VAL:O	2.17	0.44
1:L:1:MET:C	1:L:2:LYS:CG	2.85	0.44
1:F:8:ASP:O	1:F:10:THR:HG23	2.18	0.43
1:F:118:ASP:C	1:F:119:LYS:CG	2.85	0.43
1:H:11:ILE:HB	1:H:24:ILE:HD12	2.00	0.43
1:M:31:TYR:HE2	1:M:208:VAL:HA	1.83	0.43
1:B:63:PHE:HA	1:B:64:PRO:HA	1.80	0.43
1:F:149:TYR:HB3	1:F:177:MET:HG2	1.99	0.43
1:A:4:ASN:ND2	1:A:31:TYR:O	2.51	0.43
1:F:117:GLY:CA	1:F:118:ASP:HB3	2.49	0.43
1:K:161:ALA:H	1:K:183:GLY:CA	2.16	0.43
1:C:4:ASN:HB3	1:C:210:ILE:HD11	2.00	0.43
1:F:185:ALA:CB	1:F:190:ASP:HB3	2.48	0.43
1:F:203:GLY:O	1:F:204:ALA:HB2	2.18	0.43
1:G:147:ALA:CB	1:G:148:ASP:CG	2.85	0.43
1:K:207:GLY:C	1:K:208:VAL:CG1	2.86	0.43
1:M:147:ALA:O	1:M:177:MET:HE3	2.18	0.43
1:D:169:MET:O	1:D:173:VAL:HG12	2.18	0.43
1:H:160:GLY:HA3	1:H:183:GLY:HA3	2.01	0.43
1:L:48:GLU:HG3	1:L:51:LYS:HE2	2.01	0.43
1:M:2:LYS:HD2	1:M:2:LYS:HA	1.51	0.43
1:F:89:ASP:OD1	1:F:122:LYS:CD	2.46	0.43
1:H:25:LEU:HD23	1:H:36:VAL:HG11	2.01	0.43
1:I:2:LYS:HA	1:I:3:LEU:HA	1.66	0.43
1:I:206:SER:O	1:I:209:ALA:HB3	2.19	0.43
1:L:191:ALA:O	1:L:195:ILE:HG13	2.18	0.43
1:A:130:LEU:HB3	1:A:134:GLU:HB2	2.00	0.43
1:G:87:GLU:HG3	1:G:120:LEU:HB3	2.00	0.43
1:J:87:GLU:HG2	1:J:120:LEU:HB3	2.00	0.43
1:K:4:ASN:ND2	1:K:32:ASP:O	2.48	0.43
1:C:127:ALA:O	1:C:135:LYS:HE2	2.19	0.43
1:F:184:GLY:HA3	1:F:185:ALA:HA	1.67	0.43
1:D:13:LYS:O	1:D:16:THR:HG23	2.18	0.43
1:E:4:ASN:ND2	1:E:32:ASP:O	2.52	0.43
1:G:50:LEU:HD12	1:G:57:VAL:HG12	2.01	0.43
1:G:57:VAL:CG2	1:G:85:ALA:HA	2.48	0.43
1:B:18:GLN:O	1:B:21:VAL:HG22	2.18	0.43
1:B:29:LYS:HE2	1:B:49:SER:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:GLU:OE1	1:D:68:ASN:ND2	2.48	0.43
1:C:163:VAL:HG13	1:C:197:ALA:HB2	2.00	0.43
1:F:5:LYS:HD2	1:F:5:LYS:HA	1.68	0.43
1:M:92:ILE:HD12	1:M:109:ILE:HD11	2.00	0.43
1:I:51:LYS:O	1:I:52:ASP:HB2	2.19	0.42
1:E:3:LEU:HD22	1:E:188:TYR:CE1	2.54	0.42
1:F:96:ALA:HB1	1:F:101:ASN:HB3	2.01	0.42
1:J:184:GLY:HA2	1:J:185:ALA:C	2.40	0.42
1:F:11:ILE:HB	1:F:24:ILE:CD1	2.41	0.42
1:L:3:LEU:O	1:L:5:LYS:N	2.53	0.42
1:M:34:ALA:O	1:M:56:LYS:HG3	2.19	0.42
1:E:51:LYS:O	1:E:52:ASP:HB2	2.18	0.42
1:G:43:VAL:HG23	1:G:44:ALA:N	2.34	0.42
1:G:186:ARG:O	1:G:190:ASP:HB2	2.19	0.42
1:L:122:LYS:HG2	1:L:149:TYR:HB2	2.02	0.42
1:A:152:THR:HG22	1:A:169:MET:SD	2.60	0.42
1:M:4:ASN:HA	1:M:210:ILE:HD11	2.01	0.42
1:B:154:THR:O	1:B:156:PHE:HD1	2.03	0.42
1:E:61:ILE:HD12	1:E:76:GLU:HG2	2.01	0.42
1:I:151:LYS:HE3	1:I:180:LYS:HE2	2.01	0.42
1:L:78:LYS:HE3	1:L:115:ALA:CB	2.50	0.42
1:A:51:LYS:O	1:A:52:ASP:HB2	2.20	0.42
1:H:77:THR:HG23	1:H:88:ILE:HG13	2.01	0.42
1:I:173:VAL:HG22	1:I:177:MET:SD	2.60	0.42
1:A:173:VAL:CG2	1:A:177:MET:SD	3.08	0.42
1:C:122:LYS:HG2	1:C:149:TYR:HB2	2.02	0.42
1:G:68:ASN:HB3	1:G:72:VAL:CG2	2.50	0.42
1:H:57:VAL:CG2	1:H:85:ALA:HA	2.49	0.42
1:J:51:LYS:O	1:J:52:ASP:HB2	2.20	0.42
1:C:141:LEU:HD23	1:C:141:LEU:HA	1.87	0.42
1:F:170:ARG:O	1:F:174:GLY:N	2.51	0.42
1:K:59:THR:HG21	1:K:80:ALA:HB1	2.00	0.42
1:C:3:LEU:HA	1:C:3:LEU:HD12	1.76	0.42
1:E:3:LEU:HD22	1:E:188:TYR:HE1	1.85	0.42
1:E:139:CYS:SG	1:E:169:MET:HG2	2.60	0.42
1:E:206:SER:O	1:E:209:ALA:HB3	2.20	0.42
1:F:119:LYS:CB	1:F:120:LEU:HB2	2.50	0.42
1:J:77:THR:O	1:J:81:ILE:HG23	2.19	0.42
1:K:63:PHE:HA	1:K:64:PRO:HA	1.83	0.42
1:K:207:GLY:CA	1:K:208:VAL:C	2.86	0.42
1:K:209:ALA:C	1:K:211:MET:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:8:ASP:OD1	1:L:201:ARG:NH1	2.52	0.42
1:H:11:ILE:HB	1:H:24:ILE:CD1	2.50	0.41
1:K:206:SER:HB3	1:K:207:GLY:HA2	2.02	0.41
1:L:110:LYS:HA	1:L:113:VAL:HG22	2.02	0.41
1:G:110:LYS:HA	1:G:113:VAL:HG12	2.01	0.41
1:L:173:VAL:C	1:L:174:GLY:O	2.57	0.41
1:C:205:SER:O	1:C:206:SER:OG	2.22	0.41
1:D:33:PHE:HZ	1:D:207:GLY:HA2	1.86	0.41
1:L:74:ALA:O	1:L:77:THR:OG1	2.31	0.41
1:L:170:ARG:NH2	1:L:177:MET:O	2.52	0.41
1:M:3:LEU:C	1:M:5:LYS:N	2.73	0.41
1:M:31:TYR:CD1	1:M:31:TYR:N	2.89	0.41
1:M:92:ILE:CD1	1:M:109:ILE:HD11	2.50	0.41
1:M:204:ALA:HB1	1:M:206:SER:H	1.84	0.41
1:G:92:ILE:HG22	1:G:93:ASN:N	2.36	0.41
1:I:210:ILE:HD13	1:I:210:ILE:HG21	1.79	0.41
1:L:154:THR:O	1:L:156:PHE:HD1	2.02	0.41
1:M:16:THR:HA	1:M:20:GLN:OE1	2.20	0.41
1:G:2:LYS:O	1:G:4:ASN:ND2	2.54	0.41
1:I:78:LYS:NZ	1:I:115:ALA:HA	2.36	0.41
1:L:8:ASP:OD1	1:L:35:SER:OG	2.39	0.41
1:A:136:VAL:O	1:A:140:GLN:HG3	2.20	0.41
1:G:6:TYR:HE1	1:G:199:ALA:O	2.01	0.41
1:G:143:GLN:CG	1:G:143:GLN:O	2.69	0.41
1:J:151:LYS:HE3	1:J:180:LYS:HE2	2.03	0.41
1:F:151:LYS:HE2	1:F:182:SER:OG	2.20	0.41
1:G:141:LEU:C	1:G:143:GLN:N	2.73	0.41
1:L:170:ARG:HD2	1:L:198:GLY:O	2.21	0.41
1:B:60:VAL:HG12	1:B:89:ASP:HB2	2.02	0.41
1:C:63:PHE:HA	1:C:64:PRO:HA	1.94	0.41
1:D:87:GLU:HG2	1:D:120:LEU:HB3	2.03	0.41
1:E:208:VAL:HA	1:E:210:ILE:HG22	2.02	0.41
1:G:140:GLN:O	1:G:142:SER:C	2.59	0.41
1:G:162:THR:O	1:G:166:VAL:HG12	2.20	0.41
1:I:2:LYS:H	1:I:6:TYR:HE1	1.69	0.41
1:I:68:ASN:HB3	1:I:72:VAL:CG2	2.51	0.41
1:M:124:ILE:HG12	1:M:151:LYS:HB3	2.03	0.41
1:M:173:VAL:O	1:M:173:VAL:HG22	2.20	0.41
1:A:209:ALA:O	1:A:211:MET:HG2	2.20	0.41
1:D:22:GLU:OE1	1:E:23:LYS:NZ	2.47	0.41
1:D:37:CYS:HA	1:D:58:CYS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:30:GLU:HG2	1:M:31:TYR:CD1	2.56	0.41
1:M:50:LEU:HD22	1:M:55:VAL:CG1	2.51	0.41
1:B:1:MET:O	1:B:1:MET:HG2	2.21	0.40
1:B:136:VAL:CG2	1:B:168:LEU:HD21	2.50	0.40
1:E:63:PHE:CE2	1:E:64:PRO:HB3	2.56	0.40
1:F:58:CYS:HA	1:F:87:GLU:HB3	2.03	0.40
1:F:185:ALA:HB3	1:F:190:ASP:HB3	2.03	0.40
1:G:141:LEU:O	1:G:143:GLN:N	2.54	0.40
1:K:206:SER:CB	1:K:207:GLY:HA2	2.51	0.40
1:L:78:LYS:HG3	1:L:115:ALA:HB1	2.04	0.40
1:G:5:LYS:N	1:G:5:LYS:CD	2.80	0.40
1:K:207:GLY:CA	1:K:208:VAL:CB	2.99	0.40
1:A:209:ALA:C	1:A:211:MET:N	2.75	0.40
1:B:185:ALA:H	1:B:186:ARG:HG2	1.85	0.40
1:D:154:THR:O	1:D:156:PHE:HD1	2.04	0.40
1:G:143:GLN:O	1:G:143:GLN:HG2	2.21	0.40
1:K:37:CYS:HA	1:K:58:CYS:O	2.22	0.40
1:M:9:HIS:CD2	1:M:24:ILE:HG23	2.56	0.40
1:A:43:VAL:HG23	1:A:57:VAL:HG11	2.03	0.40
1:C:143:GLN:HA	1:C:177:MET:CE	2.51	0.40
1:F:87:GLU:CG	1:F:122:LYS:HE3	2.52	0.40
1:G:93:ASN:HD22	1:G:96:ALA:H	1.69	0.40
1:J:40:PRO:HA	1:J:43:VAL:HG23	2.03	0.40
1:L:207:GLY:CA	1:L:210:ILE:HG21	2.42	0.40
1:I:147:ALA:O	1:I:177:MET:HE3	2.22	0.40
1:M:3:LEU:HD23	1:M:3:LEU:HA	1.77	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	209/223 (94%)	191 (91%)	15 (7%)	3 (1%)	11 34
1	B	208/223 (93%)	191 (92%)	12 (6%)	5 (2%)	6 20
1	C	209/223 (94%)	194 (93%)	11 (5%)	4 (2%)	8 26
1	D	210/223 (94%)	189 (90%)	17 (8%)	4 (2%)	8 26
1	E	207/223 (93%)	192 (93%)	13 (6%)	2 (1%)	15 44
1	F	208/223 (93%)	177 (85%)	19 (9%)	12 (6%)	1 4
1	G	208/223 (93%)	173 (83%)	20 (10%)	15 (7%)	1 2
1	H	209/223 (94%)	198 (95%)	9 (4%)	2 (1%)	15 44
1	I	209/223 (94%)	194 (93%)	7 (3%)	8 (4%)	3 10
1	J	212/223 (95%)	193 (91%)	14 (7%)	5 (2%)	6 20
1	K	210/223 (94%)	192 (91%)	12 (6%)	6 (3%)	4 15
1	L	210/223 (94%)	188 (90%)	14 (7%)	8 (4%)	3 10
1	M	210/223 (94%)	194 (92%)	13 (6%)	3 (1%)	11 34
All	All	2719/2899 (94%)	2466 (91%)	176 (6%)	77 (3%)	5 17

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	ILE
1	B	2	LYS
1	B	185	ALA
1	D	2	LYS
1	D	207	GLY
1	E	210	ILE
1	F	114	ALA
1	F	115	ALA
1	F	176	ASP
1	G	2	LYS
1	G	145	ALA
1	G	187	SER
1	G	199	ALA
1	H	208	VAL
1	I	199	ALA
1	I	200	SER
1	K	208	VAL
1	L	208	VAL
1	M	4	ASN
1	A	127	ALA

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Mol	Chain	Res	Type
1	B	209	ALA
1	F	4	ASN
1	F	32	ASP
1	F	175	PRO
1	F	200	SER
1	F	201	ARG
1	F	206	SER
1	G	153	SER
1	G	184	GLY
1	G	207	GLY
1	I	2	LYS
1	I	209	ALA
1	J	207	GLY
1	K	101	ASN
1	K	209	ALA
1	L	3	LEU
1	M	186	ARG
1	C	205	SER
1	F	149	TYR
1	G	3	LEU
1	G	32	ASP
1	G	51	LYS
1	G	83	ASN
1	I	127	ALA
1	L	32	ASP
1	C	32	ASP
1	D	175	PRO
1	E	32	ASP
1	K	3	LEU
1	L	2	LYS
1	L	207	GLY
1	A	32	ASP
1	B	127	ALA
1	B	207	GLY
1	C	127	ALA
1	D	32	ASP
1	F	127	ALA
1	G	79	ASP
1	G	179	VAL
1	G	186	ARG
1	H	32	ASP
1	I	32	ASP

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Mol	Chain	Res	Type
1	J	32	ASP
1	J	127	ALA
1	J	175	PRO
1	K	32	ASP
1	K	210	ILE
1	L	127	ALA
1	L	175	PRO
1	F	177	MET
1	M	32	ASP
1	G	117	GLY
1	I	183	GLY
1	J	208	VAL
1	C	208	VAL
1	I	210	ILE
1	L	174	GLY

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	164/171 (96%)	162 (99%)	2 (1%)	71	92
1	B	163/171 (95%)	162 (99%)	1 (1%)	86	96
1	C	164/171 (96%)	160 (98%)	4 (2%)	49	81
1	D	165/171 (96%)	163 (99%)	2 (1%)	71	92
1	E	162/171 (95%)	159 (98%)	3 (2%)	57	85
1	F	163/171 (95%)	153 (94%)	10 (6%)	18	48
1	G	163/171 (95%)	153 (94%)	10 (6%)	18	48
1	H	164/171 (96%)	162 (99%)	2 (1%)	71	92
1	I	164/171 (96%)	159 (97%)	5 (3%)	41	75
1	J	165/171 (96%)	160 (97%)	5 (3%)	41	75
1	K	165/171 (96%)	162 (98%)	3 (2%)	59	86
1	L	165/171 (96%)	162 (98%)	3 (2%)	59	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	M	165/171 (96%)	159 (96%)	6 (4%)	35 69
All	All	2132/2223 (96%)	2076 (97%)	56 (3%)	46 79

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	176	ASP
1	B	173	VAL
1	C	1	MET
1	C	2	LYS
1	C	48	GLU
1	C	186	ARG
1	D	2	LYS
1	D	175	PRO
1	E	175	PRO
1	E	186	ARG
1	E	206	SER
1	F	37	CYS
1	F	48	GLU
1	F	57	VAL
1	F	70	PRO
1	F	116	SER
1	F	119	LYS
1	F	120	LEU
1	F	182	SER
1	F	196	GLU
1	F	201	ARG
1	G	1	MET
1	G	2	LYS
1	G	5	LYS
1	G	56	LYS
1	G	116	SER
1	G	118	ASP
1	G	141	LEU
1	G	143	GLN
1	G	173	VAL
1	G	177	MET
1	H	35	SER
1	H	104	LEU
1	I	1	MET
1	I	3	LEU

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Mol	Chain	Res	Type
1	I	173	VAL
1	I	175	PRO
1	I	176	ASP
1	J	137	LYS
1	J	175	PRO
1	J	192	ILE
1	J	196	GLU
1	J	206	SER
1	K	9	HIS
1	K	206	SER
1	K	210	ILE
1	L	1	MET
1	L	177	MET
1	L	211	MET
1	M	2	LYS
1	M	5	LYS
1	M	6	TYR
1	M	31	TYR
1	M	49	SER
1	M	56	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	9	HIS
1	G	143	GLN
1	J	9	HIS
1	J	212	ASN
1	L	101	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	211/223 (94%)	0.26	3 (1%) 75 70	57, 72, 90, 112	0
1	B	210/223 (94%)	0.47	14 (6%) 17 10	55, 68, 84, 97	0
1	C	211/223 (94%)	0.27	3 (1%) 75 70	51, 68, 90, 108	0
1	D	212/223 (95%)	0.56	18 (8%) 10 5	55, 68, 88, 109	0
1	E	209/223 (93%)	0.34	5 (2%) 59 49	52, 60, 76, 98	0
1	F	210/223 (94%)	0.55	17 (8%) 12 6	24, 81, 109, 136	0
1	G	210/223 (94%)	1.04	46 (21%) 0 0	24, 90, 111, 120	0
1	H	211/223 (94%)	0.35	2 (0%) 84 80	53, 69, 88, 99	0
1	I	211/223 (94%)	0.44	10 (4%) 31 22	58, 74, 93, 104	0
1	J	214/223 (95%)	0.38	8 (3%) 41 31	59, 79, 103, 125	0
1	K	212/223 (95%)	0.36	4 (1%) 66 59	55, 72, 90, 114	0
1	L	212/223 (95%)	0.77	23 (10%) 5 3	24, 79, 108, 131	0
1	M	212/223 (95%)	0.63	16 (7%) 14 8	25, 75, 98, 117	0
All	All	2745/2899 (94%)	0.49	169 (6%) 20 13	24, 73, 100, 136	0

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	120	LEU	7.8
1	G	1	MET	7.2
1	G	83	ASN	5.9
1	G	7	ILE	5.8
1	G	3	LEU	5.7
1	I	6	TYR	5.7
1	L	6	TYR	5.1
1	G	120	LEU	4.9
1	L	177	MET	4.7

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Mol	Chain	Res	Type	RSRZ
1	I	52	ASP	4.7
1	E	179	VAL	4.6
1	L	2	LYS	4.5
1	M	1	MET	4.3
1	F	179	VAL	4.2
1	G	86	ASP	4.2
1	L	121	VAL	4.2
1	L	142	SER	4.1
1	G	6	TYR	4.1
1	I	86	ASP	4.1
1	G	2	LYS	4.0
1	G	57	VAL	4.0
1	D	7	ILE	3.9
1	D	2	LYS	3.9
1	G	147	ALA	3.9
1	G	202	ILE	3.9
1	L	4	ASN	3.8
1	D	120	LEU	3.8
1	G	179	VAL	3.8
1	F	86	ASP	3.8
1	J	192	ILE	3.7
1	L	192	ILE	3.7
1	D	179	VAL	3.7
1	G	145	ALA	3.7
1	L	149	TYR	3.7
1	G	87	GLU	3.7
1	I	188	TYR	3.7
1	M	6	TYR	3.6
1	B	85	ALA	3.6
1	D	188	TYR	3.6
1	K	179	VAL	3.6
1	G	8	ASP	3.6
1	J	4	ASN	3.6
1	G	177	MET	3.5
1	L	1	MET	3.5
1	D	202	ILE	3.4
1	M	188	TYR	3.4
1	G	146	GLY	3.4
1	F	142	SER	3.3
1	F	193	ALA	3.3
1	J	6	TYR	3.3
1	G	113	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	176	ASP	3.3
1	B	120	LEU	3.3
1	G	31	TYR	3.3
1	G	121	VAL	3.3
1	I	50	LEU	3.2
1	F	118	ASP	3.2
1	G	34	ALA	3.2
1	M	193	ALA	3.2
1	D	173	VAL	3.1
1	D	106	LEU	3.1
1	G	188	TYR	3.1
1	L	188	TYR	3.1
1	G	201	ARG	3.1
1	M	189	GLU	3.0
1	L	88	ILE	3.0
1	G	55	VAL	3.0
1	I	51	LYS	2.9
1	L	181	ALA	2.9
1	M	176	ASP	2.9
1	G	149	TYR	2.9
1	I	74	ALA	2.9
1	I	192	ILE	2.9
1	F	192	ILE	2.9
1	G	185	ALA	2.9
1	G	35	SER	2.9
1	G	122	LYS	2.9
1	L	113	VAL	2.9
1	B	147	ALA	2.8
1	M	178	GLY	2.7
1	D	184	GLY	2.7
1	D	6	TYR	2.7
1	L	202	ILE	2.7
1	G	150	VAL	2.7
1	G	184	GLY	2.7
1	B	31	TYR	2.7
1	B	179	VAL	2.6
1	L	87	GLU	2.6
1	F	6	TYR	2.6
1	L	203	GLY	2.6
1	G	148	ASP	2.6
1	F	125	ILE	2.6
1	L	179	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	L	122	LYS	2.6
1	J	185	ALA	2.6
1	E	188	TYR	2.5
1	B	26	ALA	2.5
1	G	88	ILE	2.5
1	L	148	ASP	2.5
1	L	145	ALA	2.5
1	F	177	MET	2.5
1	G	194	PHE	2.5
1	M	56	LYS	2.5
1	C	64	PRO	2.5
1	B	188	TYR	2.5
1	G	123	VAL	2.4
1	M	212	ASN	2.4
1	K	142	SER	2.4
1	G	176	ASP	2.4
1	F	178	GLY	2.4
1	D	149	TYR	2.4
1	D	193	ALA	2.4
1	F	174	GLY	2.4
1	A	26	ALA	2.4
1	E	149	TYR	2.3
1	B	150	VAL	2.3
1	F	40	PRO	2.3
1	G	112	VAL	2.3
1	L	31	TYR	2.3
1	L	176	ASP	2.3
1	C	31	TYR	2.3
1	G	125	ILE	2.3
1	D	177	MET	2.3
1	D	142	SER	2.3
1	M	147	ALA	2.3
1	G	200	SER	2.3
1	B	145	ALA	2.3
1	G	127	ALA	2.2
1	D	200	SER	2.2
1	D	123	VAL	2.2
1	J	53	SER	2.2
1	G	199	ALA	2.2
1	M	177	MET	2.2
1	I	179	VAL	2.2
1	M	142	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	33	PHE	2.2
1	E	3	LEU	2.2
1	C	189	GLU	2.2
1	G	109	ILE	2.2
1	G	187	SER	2.2
1	J	34	ALA	2.2
1	G	41	THR	2.2
1	A	188	TYR	2.1
1	K	181	ALA	2.1
1	I	5	LYS	2.1
1	B	57	VAL	2.1
1	B	88	ILE	2.1
1	G	191	ALA	2.1
1	B	6	TYR	2.1
1	B	144	GLU	2.1
1	F	194	PHE	2.1
1	F	119	LYS	2.1
1	M	11	ILE	2.1
1	D	146	GLY	2.1
1	M	203	GLY	2.1
1	J	30	GLU	2.1
1	K	2	LYS	2.1
1	B	177	MET	2.1
1	E	177	MET	2.1
1	J	64	PRO	2.1
1	G	4	ASN	2.1
1	D	3	LEU	2.0
1	F	85	ALA	2.0
1	M	169	MET	2.0
1	H	147	ALA	2.0
1	M	181	ALA	2.0
1	A	3	LEU	2.0
1	F	175	PRO	2.0
1	H	57	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.