



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 24, 2023 – 11:13 AM EST

PDB ID : 3LYC
Title : Crystal structure of Putative pectinase (YP_001304412.1) from Parabacteroides distasonis ATCC 8503 at 2.30 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2010-02-26
Resolution : 2.30 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.2
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) : 2.31.2

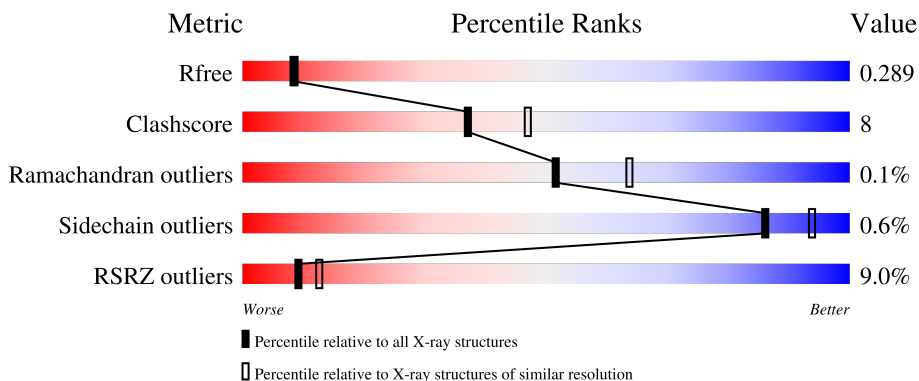
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 $\leq 5\%$. 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	241	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> </div> <p style="margin-left: 20px;">87% 12% .</p>
1	B	241	<div style="display: flex; align-items: center;"> <div style="width: 17%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> </div> <p style="margin-left: 20px;">17% 81% 17% .</p>
1	C	241	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> </div> <p style="margin-left: 20px;">2% 87% 13%</p>
1	D	241	<div style="display: flex; align-items: center;"> <div style="width: 15%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> </div> <p style="margin-left: 20px;">15% 86% 13%</p>
1	E	241	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> </div> <p style="margin-left: 20px;">3% 87% 13%</p>

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Mol	Chain	Length	Quality of chain
1	F	241	<p>17% 88% 11%</p>
1	G	241	<p>2% 86% 14%</p>
1	H	241	<p>12% 84% 16%</p>
1	I	241	<p>4% 87% 12%</p>
1	J	241	<p>17% 84% 15%</p>
1	K	241	<p>2% 89% 11%</p>
1	L	241	<p>12% 80% 17%</p>
1	M	241	<p>5% 83% 17%</p>
1	N	241	<p>16% 88% 10%</p>
1	O	241	<p>1% 86% 14%</p>
1	P	241	<p>15% 80% 17%</p>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 29713 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 Putative pectinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	241	Total 1831	C 1142	N 307	O 371	S 6	Se 5	0	7	0
1	B	237	Total 1785	C 1122	N 293	O 361	S 4	Se 5	0	3	0
1	C	241	Total 1831	C 1148	N 305	O 368	S 4	Se 6	0	8	0
1	D	240	Total 1780	C 1116	N 299	O 356	S 4	Se 5	0	4	0
1	E	241	Total 1836	C 1147	N 310	O 369	S 5	Se 5	0	5	0
1	F	239	Total 1782	C 1117	N 294	O 362	S 4	Se 5	0	4	0
1	G	241	Total 1811	C 1134	N 303	O 365	S 4	Se 5	0	5	0
1	H	241	Total 1822	C 1143	N 297	O 373	S 4	Se 5	0	6	0
1	I	241	Total 1811	C 1134	N 297	O 369	S 6	Se 5	0	5	0
1	J	238	Total 1809	C 1134	N 302	O 364	S 4	Se 5	0	7	0
1	K	241	Total 1816	C 1132	N 305	O 369	S 4	Se 6	0	5	0
1	L	235	Total 1746	C 1096	N 287	O 354	S 4	Se 5	0	6	0
1	M	241	Total 1862	C 1169	N 309	O 373	S 6	Se 5	0	10	0
1	N	238	Total 1824	C 1141	N 306	O 368	S 4	Se 5	0	7	0
1	O	240	Total 1836	C 1149	N 306	O 372	S 4	Se 5	0	7	0
1	P	232	Total 1681	C 1053	N 276	O 343	S 4	Se 5	0	1	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A6LGH6
B	0	GLY	-	expression tag	UNP A6LGH6
C	0	GLY	-	expression tag	UNP A6LGH6
D	0	GLY	-	expression tag	UNP A6LGH6
E	0	GLY	-	expression tag	UNP A6LGH6
F	0	GLY	-	expression tag	UNP A6LGH6
G	0	GLY	-	expression tag	UNP A6LGH6
H	0	GLY	-	expression tag	UNP A6LGH6
I	0	GLY	-	expression tag	UNP A6LGH6
J	0	GLY	-	expression tag	UNP A6LGH6
K	0	GLY	-	expression tag	UNP A6LGH6
L	0	GLY	-	expression tag	UNP A6LGH6
M	0	GLY	-	expression tag	UNP A6LGH6
N	0	GLY	-	expression tag	UNP A6LGH6
O	0	GLY	-	expression tag	UNP A6LGH6
P	0	GLY	-	expression tag	UNP A6LGH6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	90	Total O 90 90	0	0
2	B	38	Total O 38 38	0	0
2	C	50	Total O 50 50	0	0
2	D	21	Total O 21 21	0	0
2	E	97	Total O 97 97	0	0
2	F	46	Total O 46 46	0	0
2	G	64	Total O 64 64	0	0
2	H	24	Total O 24 24	0	0
2	I	84	Total O 84 84	0	0
2	J	50	Total O 50 50	0	0
2	K	55	Total O 55 55	0	0

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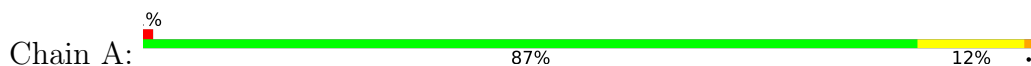
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	L	17	Total O 17 17	0	0
2	M	88	Total O 88 88	0	0
2	N	39	Total O 39 39	0	0
2	O	63	Total O 63 63	0	0
2	P	24	Total O 24 24	0	0

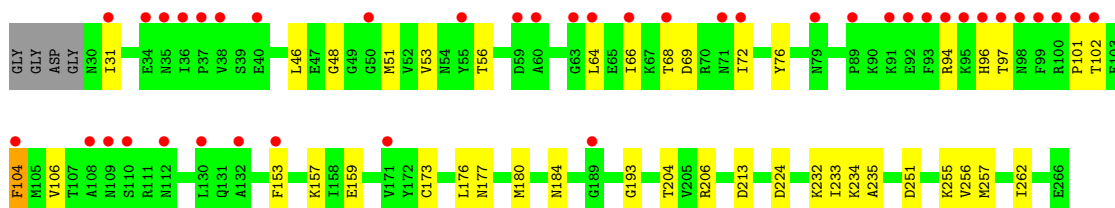
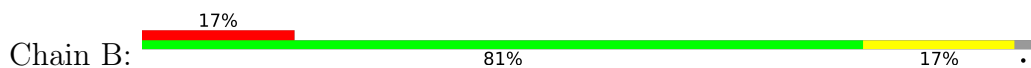
3 Residue-property plots [i](#)

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.

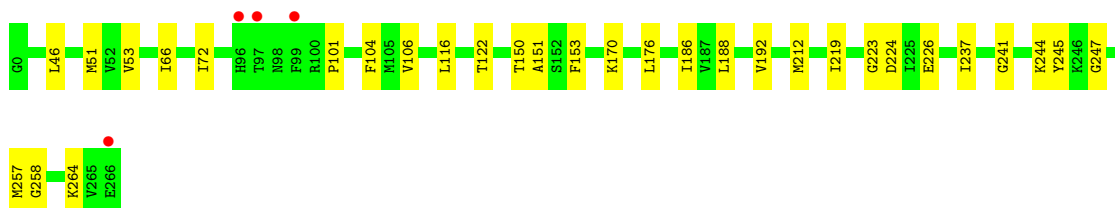
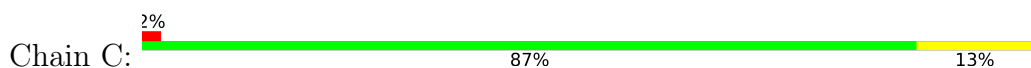
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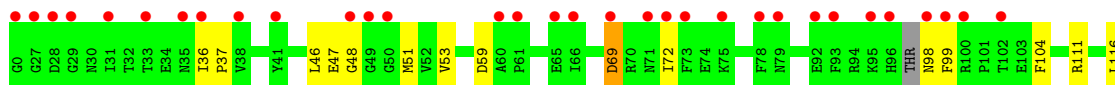
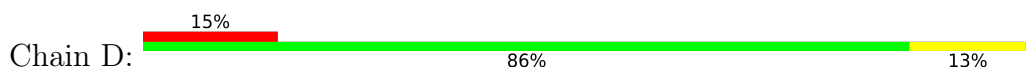
- Molecule 1: Putative pectinase



- Molecule 1: Putative pectinase

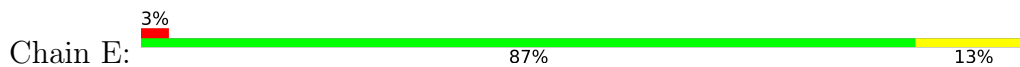


- Molecule 1: Putative pectinase

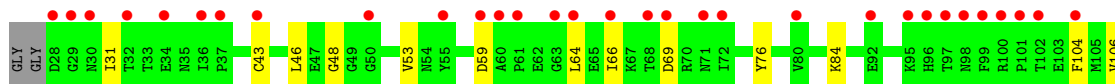
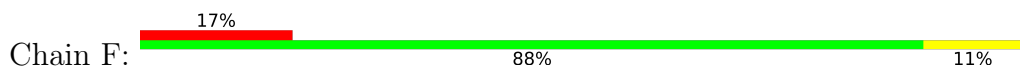




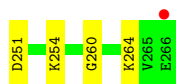
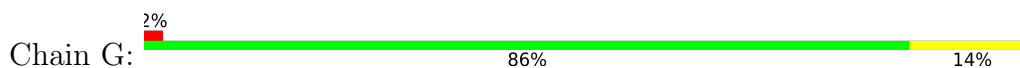
- Molecule 1: Putative pectinase



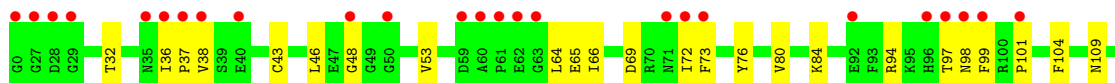
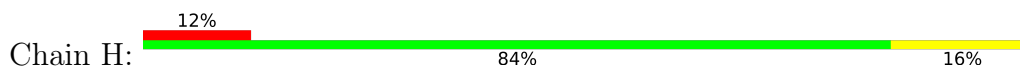
- Molecule 1: Putative pectinase



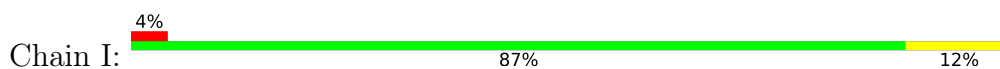
- Molecule 1: Putative pectinase

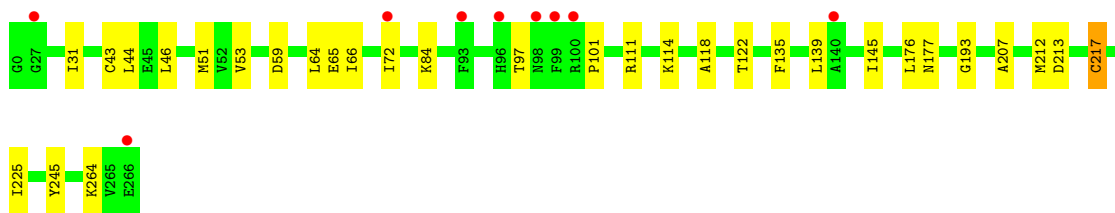


- Molecule 1: Putative pectinase

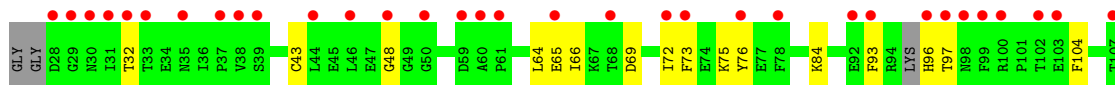
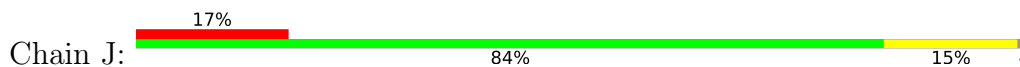


- Molecule 1: Putative pectinase

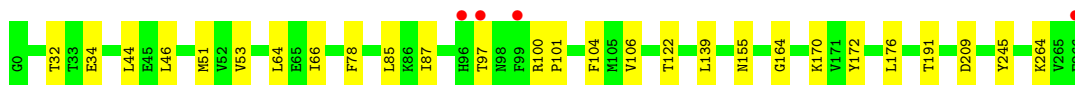
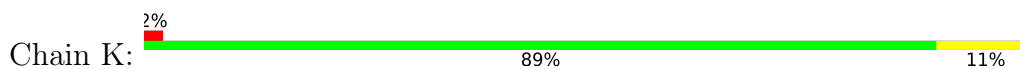




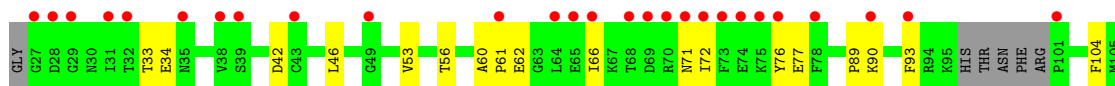
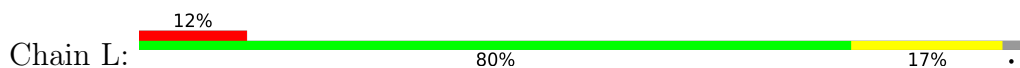
- Molecule 1: Putative pectinase



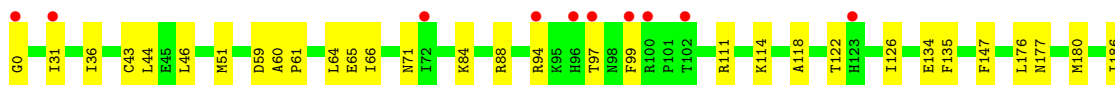
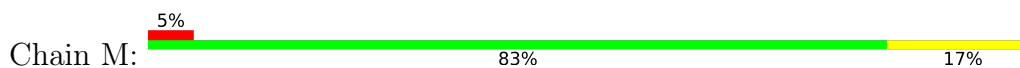
- Molecule 1: Putative pectinase



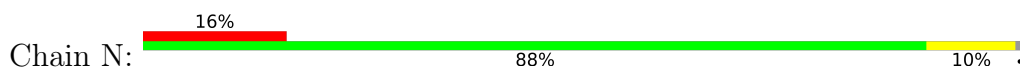
- Molecule 1: Putative pectinase

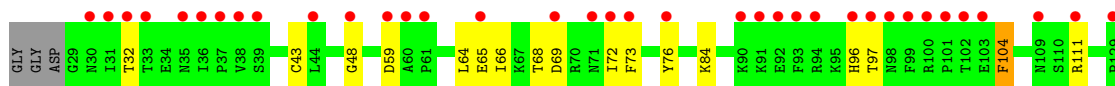


- Molecule 1: Putative pectinase

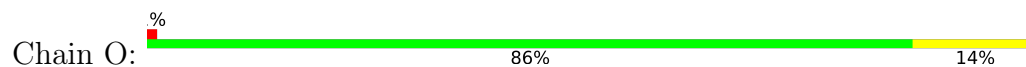


- Molecule 1: Putative pectinase

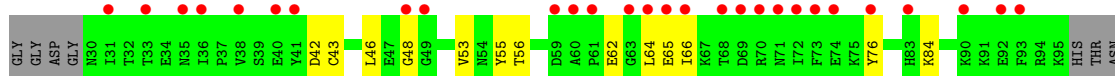
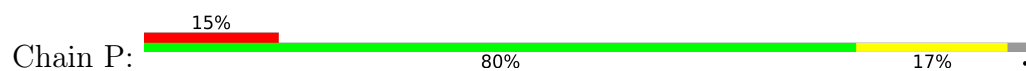




- Molecule 1: Putative pectinase



- Molecule 1: Putative pectinase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.12Å 104.61Å 393.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.51 – 2.30 49.53 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.5 (49.51-2.30) 97.5 (49.53-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.5.0102, PHENIX	Depositor
R, R_{free}	0.244 , 0.280 0.253 , 0.289	Depositor DCC
R_{free} test set	9370 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtrriage
Anisotropy	0.333	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.000 for k,h,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	29713	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 62.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0466e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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](#)

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	0.64	0/1872	0.46	0/2510
1	B	0.56	0/1815	0.45	0/2435
1	C	0.58	0/1876	0.44	0/2515
1	D	0.51	0/1812	0.43	0/2431
1	E	0.66	0/1873	0.46	0/2511
1	F	0.54	0/1815	0.44	0/2439
1	G	0.58	0/1847	0.45	0/2477
1	H	0.53	0/1862	0.43	0/2500
1	I	0.66	2/1847 (0.1%)	0.45	0/2479
1	J	0.52	0/1848	0.43	0/2479
1	K	0.58	0/1851	0.45	0/2483
1	L	0.52	0/1783	0.43	0/2393
1	M	0.66	0/1915	0.46	0/2565
1	N	0.56	0/1868	0.43	0/2508
1	O	0.60	0/1879	0.45	0/2515
1	P	0.50	0/1702	0.43	0/2291
All	All	0.58	2/29465 (0.0%)	0.44	0/39531

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	217[A]	CYS	CB-SG	-5.15	1.73	1.81
1	I	217[B]	CYS	CB-SG	-5.15	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1831	0	1786	34	0
1	B	1785	0	1730	32	0
1	C	1831	0	1791	24	0
1	D	1780	0	1711	24	0
1	E	1836	0	1792	27	0
1	F	1782	0	1703	18	0
1	G	1811	0	1757	24	0
1	H	1822	0	1744	28	0
1	I	1811	0	1749	33	0
1	J	1809	0	1751	27	0
1	K	1816	0	1768	31	0
1	L	1746	0	1678	27	0
1	M	1862	0	1833	41	0
1	N	1824	0	1768	30	0
1	O	1836	0	1799	31	0
1	P	1681	0	1573	28	0
2	A	90	0	0	1	0
2	B	38	0	0	1	0
2	C	50	0	0	0	0
2	D	21	0	0	0	0
2	E	97	0	0	1	0
2	F	46	0	0	0	0
2	G	64	0	0	1	0
2	H	24	0	0	0	0
2	I	84	0	0	0	0
2	J	50	0	0	2	0
2	K	55	0	0	0	0
2	L	17	0	0	0	0
2	M	88	0	0	1	0
2	N	39	0	0	0	0
2	O	63	0	0	1	0
2	P	24	0	0	0	0
All	All	29713	0	27933	443	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 8.

All (443) 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:K:46:LEU:HD23	1:K:51:MSE:CE	1.88	1.04
1:I:46:LEU:CD2	1:I:51:MSE:HE1	1.89	1.02
1:C:46:LEU:HD22	1:C:51:MSE:HE1	1.43	1.00
1:O:46:LEU:HB3	1:O:51:MSE:HE1	1.44	1.00
1:N:72:ILE:HD11	1:N:104:PHE:CZ	2.00	0.97
1:K:46:LEU:CD2	1:K:51:MSE:HE2	1.95	0.97
1:N:72:ILE:HD11	1:N:104:PHE:CE2	2.00	0.96
1:I:46:LEU:HD23	1:I:51:MSE:HE1	1.43	0.96
1:E:46:LEU:HD13	1:E:53:VAL:HG21	1.50	0.93
1:A:46:LEU:HD23	1:A:51:MSE:HE1	1.51	0.92
1:L:56:THR:HG23	1:L:128:SER:HB3	1.53	0.90
1:F:66:ILE:HD12	1:F:106:VAL:HG22	1.57	0.87
1:A:46:LEU:CD2	1:A:51:MSE:HE1	2.05	0.87
1:M:46:LEU:CD2	1:M:51:MSE:HE1	2.05	0.87
1:E:46:LEU:HD22	1:E:51:MSE:HE1	1.58	0.86
1:N:68:THR:OG1	1:N:72:ILE:HG21	1.77	0.85
1:G:46:LEU:HB3	1:G:51:MSE:HE1	1.57	0.84
1:K:46:LEU:HD23	1:K:51:MSE:HE2	1.53	0.84
1:K:51:MSE:HB3	1:K:122:THR:HG22	1.60	0.83
1:H:38:VAL:HG13	1:H:80:VAL:HG21	1.61	0.83
1:H:97:THR:HG22	1:H:98:ASN:H	1.44	0.81
1:B:72:ILE:HD11	1:B:101:PRO:HG3	1.62	0.81
1:N:72:ILE:CD1	1:N:104:PHE:CE2	2.63	0.81
1:P:56:THR:HG23	1:P:128:SER:HB3	1.63	0.80
1:J:48:GLY:HA2	1:J:76:TYR:OH	1.84	0.78
1:D:180:MSE:HE3	1:D:199:ILE:HG12	1.64	0.78
1:K:46:LEU:CD2	1:K:51:MSE:CE	2.59	0.75
1:M:46:LEU:HD23	1:M:51:MSE:HE1	1.68	0.75
1:K:46:LEU:HB3	1:K:51:MSE:HE1	1.68	0.75
1:O:265:VAL:O	1:O:266:GLU:HG3	1.87	0.74
1:J:69:ASP:OD1	1:J:72:ILE:HD13	1.88	0.74
1:J:250[A]:GLN:NE2	1:K:97:THR:HG23	2.03	0.74
1:K:46:LEU:HD22	1:K:51:MSE:HE2	1.69	0.72
1:B:46:LEU:HD13	1:B:53:VAL:HG21	1.73	0.71
1:M:65:GLU:C	1:M:66:ILE:HD12	2.12	0.70
1:I:97:THR:HG22	1:I:97:THR:O	1.91	0.70
1:A:96:HIS:C	1:A:98:ASN:H	1.94	0.70
1:A:95:LYS:O	1:A:96:HIS:CB	2.40	0.70
1:F:48:GLY:HA2	1:F:76:TYR:OH	1.91	0.69
1:N:68:THR:HG21	1:N:72:ILE:HD13	1.74	0.69
1:K:46:LEU:HB3	1:K:51:MSE:CE	2.23	0.69
1:F:176:LEU:HD23	1:F:177:ASN:N	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:176:LEU:HD23	1:M:177:ASN:N	2.08	0.68
1:O:46:LEU:HD13	1:O:53:VAL:HG21	1.76	0.68
1:J:191:THR:HG22	2:J:306:HOH:O	1.93	0.68
1:M:180:MSE:HE2	1:M:186:ILE:HD12	1.76	0.68
1:I:46:LEU:CD2	1:I:51:MSE:CE	2.69	0.67
1:P:144:ILE:HD12	1:P:165:ASP:HB2	1.76	0.67
1:J:66:ILE:N	1:J:66:ILE:HD12	2.10	0.66
1:I:65:GLU:C	1:I:66:ILE:HD12	2.16	0.66
1:M:46:LEU:HD22	1:M:51:MSE:HE1	1.78	0.66
1:B:66:ILE:HD12	1:B:106:VAL:HG22	1.78	0.66
1:I:46:LEU:HD22	1:I:51:MSE:HE1	1.75	0.66
1:A:97:THR:HG22	1:A:97:THR:O	1.96	0.65
1:L:60:ALA:HB1	1:L:61:PRO:HD2	1.76	0.65
1:O:46:LEU:CB	1:O:51:MSE:HE1	2.25	0.65
1:M:66:ILE:HD12	1:M:66:ILE:N	2.12	0.64
1:F:64:LEU:HD11	1:F:66:ILE:HD11	1.79	0.64
1:H:66:ILE:N	1:H:66:ILE:HD12	2.11	0.64
1:I:176:LEU:C	1:I:176:LEU:HD23	2.18	0.64
1:B:48:GLY:HA3	1:B:51:MSE:HE3	1.78	0.64
1:N:48:GLY:HA2	1:N:76:TYR:OH	1.97	0.64
1:P:66:ILE:HD12	1:P:66:ILE:N	2.12	0.63
1:D:265:VAL:CG1	1:F:266:GLU:HG2	2.29	0.63
1:B:68:THR:OG1	1:B:72:ILE:HD12	1.98	0.63
1:J:246:LYS:HG2	1:J:265:VAL:HG23	1.80	0.63
1:O:46:LEU:CD2	1:O:87:ILE:HD12	2.29	0.62
1:E:65:GLU:C	1:E:66:ILE:HD12	2.20	0.62
1:H:32:THR:HG23	1:H:73:PHE:CE2	2.34	0.62
1:I:46:LEU:HD23	1:I:51:MSE:CE	2.23	0.62
1:J:65:GLU:C	1:J:66:ILE:HD12	2.19	0.62
1:O:46:LEU:HD23	1:O:87:ILE:HB	1.79	0.62
1:H:94:ARG:HG2	1:H:94:ARG:HH11	1.64	0.62
1:F:176:LEU:HD23	1:F:176:LEU:C	2.21	0.62
1:N:235:ALA:HB3	1:N:262:ILE:HD13	1.81	0.61
1:E:97:THR:HG22	1:E:97:THR:O	2.01	0.60
1:P:48:GLY:HA2	1:P:76:TYR:OH	2.02	0.60
1:D:69:ASP:HB2	1:D:72:ILE:HD13	1.84	0.60
1:D:144:ILE:N	1:D:144:ILE:HD12	2.17	0.60
1:C:66:ILE:CD1	1:C:106:VAL:HG22	2.32	0.60
1:L:206:ARG:NH2	1:O:102:THR:HG23	2.16	0.60
1:L:66:ILE:HD12	1:L:106:VAL:HG22	1.84	0.60
1:H:235:ALA:HB3	1:H:262:ILE:HD13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:LEU:C	1:B:176:LEU:HD23	2.22	0.59
1:A:46:LEU:HD22	1:A:53:VAL:HG21	1.85	0.59
1:B:235:ALA:HB3	1:B:262:ILE:HD13	1.84	0.59
1:N:72:ILE:HD12	1:N:104:PHE:CD2	2.38	0.59
1:B:157:LYS:CE	1:B:159:GLU:OE2	2.51	0.58
1:E:46:LEU:HB3	1:E:51:MSE:HE1	1.85	0.58
1:H:97:THR:HG22	1:H:98:ASN:N	2.16	0.58
1:J:32:THR:HG23	1:J:73:PHE:CE2	2.38	0.58
1:H:48:GLY:HA2	1:H:76:TYR:OH	2.04	0.58
1:L:235:ALA:HB3	1:L:262:ILE:HD13	1.84	0.58
1:B:48:GLY:HA2	1:B:76:TYR:OH	2.04	0.58
1:D:176:LEU:C	1:D:176:LEU:HD23	2.24	0.58
1:G:46:LEU:CD2	1:G:87:ILE:HD12	2.33	0.58
1:O:176:LEU:C	1:O:176:LEU:HD23	2.24	0.57
1:L:42:ASP:O	1:L:113:LEU:HD12	2.03	0.57
1:I:46:LEU:HD22	1:I:51:MSE:CE	2.32	0.57
1:M:36:ILE:CG1	1:M:66:ILE:HD13	2.34	0.57
1:E:46:LEU:CD1	1:E:53:VAL:HG21	2.30	0.57
1:J:250[A]:GLN:HA	1:J:250[A]:GLN:OE1	2.05	0.57
1:M:36:ILE:HG12	1:M:66:ILE:HD13	1.87	0.57
1:M:46:LEU:HD22	1:M:51:MSE:CE	2.34	0.57
1:N:59:ASP:O	1:N:111[A]:ARG:NH1	2.37	0.57
1:N:68:THR:HG23	1:N:72:ILE:HG23	1.87	0.57
1:A:96:HIS:C	1:A:98:ASN:N	2.58	0.57
1:M:134:GLU:HB2	2:M:818:HOH:O	2.05	0.57
1:L:71:ASN:OD1	1:L:72:ILE:N	2.38	0.57
1:I:118:ALA:HB1	1:I:122:THR:HG21	1.85	0.56
1:M:176:LEU:HD23	1:M:176:LEU:C	2.25	0.56
1:C:219:ILE:HD13	1:C:223:GLY:HA3	1.87	0.56
1:M:217[B]:CYS:SG	1:M:225:ILE:HD12	2.45	0.56
1:O:46:LEU:HD21	1:O:87:ILE:HD12	1.87	0.56
1:A:176:LEU:HD23	1:A:176:LEU:C	2.26	0.56
1:C:244[A]:LYS:HB2	1:C:244[A]:LYS:NZ	2.21	0.56
1:I:66:ILE:HD12	1:I:66:ILE:N	2.21	0.56
1:J:32:THR:HG23	1:J:73:PHE:HE2	1.71	0.56
1:P:176:LEU:C	1:P:176:LEU:HD23	2.26	0.56
1:G:176:LEU:C	1:G:176:LEU:HD23	2.26	0.56
1:J:253[A]:GLN:OE1	1:L:253[A]:GLN:NE2	2.39	0.56
1:G:46:LEU:HD23	1:G:87:ILE:HB	1.86	0.56
1:I:31:ILE:N	1:I:31:ILE:HD12	2.21	0.56
1:K:209:ASP:CG	1:O:170:LYS:HZ2	2.10	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:176:LEU:HD23	1:O:177:ASN:N	2.21	0.56
1:H:32:THR:HG23	1:H:73:PHE:HE2	1.70	0.56
1:H:46:LEU:HD13	1:H:53:VAL:HG21	1.87	0.55
1:J:204:THR:HG23	1:J:206[B]:ARG:NH1	2.21	0.55
1:N:72:ILE:CD1	1:N:104:PHE:CD2	2.89	0.55
1:K:46:LEU:HD23	1:K:51:MSE:HE1	1.82	0.55
1:O:232:LYS:HG2	1:O:251:ASP:HB3	1.87	0.55
1:H:99:PHE:O	1:H:101:PRO:HD3	2.07	0.55
1:L:56:THR:HG23	1:L:128:SER:CB	2.29	0.55
1:I:46:LEU:HB3	1:I:51:MSE:HE1	1.88	0.55
1:C:176:LEU:HD23	1:C:176:LEU:C	2.28	0.54
1:G:232[B]:LYS:HD2	1:G:251:ASP:OD2	2.07	0.54
1:O:235:ALA:HB3	1:O:262:ILE:HD11	1.90	0.54
1:B:31:ILE:HD13	1:B:69[B]:ASP:OD1	2.06	0.54
1:M:64:LEU:HG	1:M:66:ILE:HD11	1.89	0.54
1:C:244[A]:LYS:HB2	1:C:244[A]:LYS:HZ3	1.72	0.54
1:F:43:CYS:HB2	1:F:84:LYS:HG2	1.89	0.54
1:J:64:LEU:HG	1:J:66:ILE:HD11	1.90	0.54
1:A:59:ASP:OD1	1:A:111[A]:ARG:NH1	2.41	0.54
1:K:176:LEU:C	1:K:176:LEU:HD23	2.28	0.54
1:A:46:LEU:CD2	1:A:51:MSE:CE	2.83	0.54
1:A:193:GLY:O	1:A:213:ASP:HB2	2.07	0.54
1:H:94:ARG:HG2	1:H:94:ARG:NH1	2.23	0.54
1:M:59:ASP:OD1	1:M:111[A]:ARG:NH1	2.41	0.53
1:P:42:ASP:O	1:P:113:LEU:HD12	2.08	0.53
1:E:72:ILE:HD12	1:E:101:PRO:HB3	1.89	0.53
1:I:217[B]:CYS:SG	1:I:225:ILE:CD1	2.97	0.53
1:N:176:LEU:C	1:N:176:LEU:HD23	2.29	0.53
1:K:66:ILE:CD1	1:K:106:VAL:HG22	2.38	0.53
1:P:62:GLU:OE1	1:P:62:GLU:N	2.39	0.53
1:B:176:LEU:HD23	1:B:177:ASN:N	2.23	0.53
1:F:153:PHE:O	1:F:173:CYS:HA	2.08	0.52
1:H:180:MSE:SE	1:H:186:ILE:HD12	2.59	0.52
1:E:46:LEU:HD23	1:E:87:ILE:HB	1.91	0.52
1:C:51:MSE:HB2	1:C:122:THR:HG22	1.92	0.52
1:D:46:LEU:HD13	1:D:53:VAL:HG21	1.92	0.52
1:F:248[B]:ASP:OD1	1:F:264:LYS:NZ	2.41	0.52
1:H:224:ASP:C	1:H:224:ASP:OD1	2.48	0.52
1:D:204:THR:HG23	1:D:206[B]:ARG:NH1	2.25	0.52
1:M:180:MSE:HE2	1:M:186:ILE:CD1	2.39	0.52
1:P:218:LYS:HD3	1:P:236:GLU:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:LEU:HD11	1:B:66:ILE:HD11	1.92	0.52
1:N:196[A]:GLU:HA	1:N:216:GLU:O	2.10	0.52
1:N:196[B]:GLU:HA	1:N:216:GLU:O	2.10	0.52
1:H:69:ASP:HB2	1:H:72:ILE:HG12	1.92	0.52
1:C:151:ALA:HB1	1:C:153:PHE:CE2	2.44	0.52
1:F:235:ALA:HB3	1:F:262:ILE:HD13	1.91	0.52
1:P:180:MSE:SE	1:P:186:ILE:HD12	2.60	0.52
1:G:31:ILE:N	1:G:31:ILE:HD12	2.26	0.51
1:A:46:LEU:HD22	1:A:53:VAL:CG2	2.41	0.51
1:K:44:LEU:HG	1:K:46:LEU:HD11	1.91	0.51
1:A:132:ALA:O	1:A:153:PHE:HA	2.11	0.51
1:K:209:ASP:OD1	1:O:170:LYS:NZ	2.44	0.51
1:P:247:GLY:O	1:P:264:LYS:NZ	2.43	0.51
1:A:176:LEU:HD23	1:A:177:ASN:N	2.25	0.51
1:N:66:ILE:HD12	1:N:66:ILE:N	2.25	0.51
1:M:217[B]:CYS:SG	1:M:225:ILE:CD1	2.98	0.51
1:N:72:ILE:HD12	1:N:104:PHE:CE2	2.45	0.51
1:G:46:LEU:HD13	1:G:53:VAL:HG21	1.92	0.51
1:O:31:ILE:HD12	1:O:31:ILE:N	2.26	0.51
1:A:97:THR:HB	1:B:257:MSE:HA	1.92	0.51
1:L:33:THR:HG22	1:L:34:GLU:N	2.25	0.51
1:C:116:LEU:C	1:C:116:LEU:HD23	2.31	0.50
1:G:176:LEU:HD23	1:G:177:ASN:N	2.26	0.50
1:K:46:LEU:HD22	1:K:53:VAL:HG21	1.94	0.50
1:M:46:LEU:CD2	1:M:51:MSE:CE	2.85	0.50
1:M:193:GLY:O	1:M:213:ASP:HB2	2.12	0.50
1:D:143:GLY:C	1:D:144:ILE:HD12	2.32	0.50
1:M:88:ARG:HD2	1:M:94:ARG:NH2	2.26	0.50
1:L:119:ALA:HA	1:L:140:ALA:O	2.12	0.50
1:N:32:THR:HG23	1:N:73:PHE:CE2	2.47	0.50
1:D:116:LEU:HD21	1:D:124:VAL:HG11	1.94	0.49
1:E:193:GLY:O	1:E:213:ASP:HB2	2.13	0.49
1:I:72:ILE:HD12	1:I:101:PRO:HB3	1.93	0.49
1:P:144:ILE:CD1	1:P:165:ASP:HB2	2.42	0.49
1:D:180:MSE:CE	1:D:199:ILE:HG12	2.39	0.49
1:E:176:LEU:C	1:E:176:LEU:HD23	2.32	0.49
1:M:46:LEU:HB3	1:M:51:MSE:HE1	1.93	0.49
1:J:66:ILE:N	1:J:66:ILE:CD1	2.76	0.49
1:B:72:ILE:HD13	1:B:104:PHE:CD2	2.47	0.49
1:J:75:LYS:HG2	1:J:93:PHE:CD1	2.48	0.49
1:P:64:LEU:HG	1:P:66:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:LEU:CD2	1:E:87:ILE:HD12	2.43	0.49
1:E:237:ILE:HD13	1:E:241:GLY:HA3	1.94	0.49
1:I:46:LEU:HD22	1:I:53:VAL:HG21	1.95	0.49
1:I:217[B]:CYS:SG	1:I:225:ILE:HD12	2.53	0.49
1:C:226:GLU:HG2	1:C:244[A]:LYS:HZ3	1.78	0.48
1:E:31:ILE:N	1:E:31:ILE:HD12	2.26	0.48
1:K:44:LEU:HD13	1:K:85:LEU:HD23	1.95	0.48
1:L:46:LEU:HD13	1:L:53:VAL:HG21	1.95	0.48
1:N:68:THR:HG23	1:N:72:ILE:CG2	2.43	0.48
1:H:254[B]:LYS:HD2	1:H:262:ILE:HB	1.95	0.48
1:C:46:LEU:HD13	1:C:53:VAL:HG21	1.95	0.48
1:G:66:ILE:HG13	1:G:78:PHE:CE2	2.48	0.48
1:I:176:LEU:HD23	1:I:177:ASN:N	2.28	0.48
1:J:48:GLY:CA	1:J:76:TYR:OH	2.59	0.48
1:B:153:PHE:O	1:B:173:CYS:HA	2.14	0.48
1:E:59:ASP:OD1	1:E:111[A]:ARG:NH1	2.47	0.48
1:F:176:LEU:C	1:F:176:LEU:CD2	2.82	0.48
1:I:43[B]:CYS:HB3	1:I:84:LYS:HA	1.96	0.48
1:P:43:CYS:HB2	1:P:84:LYS:HG2	1.95	0.48
1:I:44:LEU:HG	1:I:46:LEU:HD11	1.95	0.48
1:H:176:LEU:HD23	1:H:176:LEU:C	2.34	0.48
1:J:235:ALA:HB3	1:J:262:ILE:HD13	1.95	0.48
1:L:233:ILE:CG2	1:L:252:ILE:HG23	2.44	0.48
1:N:69:ASP:HB2	1:N:72:ILE:HG22	1.95	0.48
1:I:59:ASP:O	1:I:111[A]:ARG:CZ	2.62	0.47
1:K:32:THR:HG22	1:K:34:GLU:HG2	1.94	0.47
1:M:44:LEU:HG	1:M:46:LEU:HD11	1.95	0.47
1:A:44:LEU:HG	1:A:46:LEU:HD11	1.95	0.47
1:A:97:THR:HB	1:B:256:VAL:O	2.15	0.47
1:K:172:TYR:HA	1:K:191:THR:O	2.14	0.47
1:J:176:LEU:C	1:J:176:LEU:HD23	2.35	0.47
1:M:126:ILE:HG13	1:M:147:PHE:CD1	2.50	0.47
1:E:46:LEU:HD22	1:E:51:MSE:CE	2.38	0.47
1:G:192:VAL:O	1:G:212:MSE:HA	2.14	0.47
1:I:59:ASP:O	1:I:111[A]:ARG:NH1	2.47	0.47
1:P:196:GLU:HA	1:P:216:GLU:O	2.14	0.47
1:C:72:ILE:HD12	1:C:101:PRO:HB3	1.97	0.47
1:D:235:ALA:HB3	1:D:262:ILE:HD13	1.97	0.47
1:N:68:THR:CG2	1:N:72:ILE:CG2	2.92	0.47
1:A:55:TYR:CZ	1:A:113:LEU:HD22	2.50	0.47
1:H:38:VAL:HG21	1:H:64:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:192:VAL:HG23	1:H:210:CYS:SG	2.55	0.47
1:L:77:GLU:HB3	1:L:90:LYS:HG2	1.97	0.47
1:M:64:LEU:HG	1:M:66:ILE:CD1	2.44	0.47
1:P:65:GLU:C	1:P:66:ILE:HD12	2.35	0.47
1:O:29:GLY:O	1:O:31:ILE:HD12	2.14	0.47
1:L:176:LEU:C	1:L:176:LEU:HD23	2.35	0.46
1:B:96:HIS:O	1:B:97:THR:OG1	2.28	0.46
1:B:224:ASP:OD1	1:B:224:ASP:C	2.54	0.46
1:K:139:LEU:HD23	1:K:164:GLY:HA3	1.97	0.46
1:F:46:LEU:HD13	1:F:53:VAL:HG21	1.97	0.46
1:A:46:LEU:HD22	1:A:51:MSE:HE1	1.94	0.46
1:H:224:ASP:OD1	1:H:225:ILE:N	2.48	0.46
1:J:125:ASN:ND2	2:J:401:HOH:O	2.35	0.46
1:L:180:MSE:HE3	1:L:199:ILE:HG12	1.97	0.46
1:I:72:ILE:CD1	1:I:101:PRO:HB3	2.45	0.46
1:J:245:TYR:OH	1:J:252:ILE:HD13	2.16	0.46
1:C:66:ILE:HD13	1:C:106:VAL:HG22	1.98	0.46
1:P:186:ILE:HG22	1:P:188:LEU:HG	1.97	0.46
1:K:78:PHE:CD2	1:K:87:ILE:HG23	2.50	0.46
1:M:66:ILE:N	1:M:66:ILE:CD1	2.78	0.46
1:M:97:THR:HA	1:M:99[B]:PHE:CE2	2.51	0.46
1:M:235:ALA:O	1:M:254:LYS:HA	2.16	0.46
1:C:237:ILE:HD13	1:C:241:GLY:HA3	1.98	0.46
1:G:122:THR:O	1:G:143:GLY:HA3	2.15	0.46
1:I:59:ASP:OD1	1:I:111[A]:ARG:NH1	2.49	0.46
1:J:245:TYR:CE1	1:J:264:LYS:HB2	2.51	0.46
1:L:197:PHE:O	1:L:217:CYS:HA	2.16	0.46
1:A:94:ARG:C	1:A:96:HIS:H	2.18	0.45
1:B:193:GLY:O	1:B:213:ASP:HB2	2.15	0.45
1:E:116:LEU:HD23	1:E:116:LEU:C	2.36	0.45
1:K:64:LEU:HD11	1:K:106:VAL:HG13	1.98	0.45
1:P:46:LEU:HD13	1:P:53:VAL:HG21	1.98	0.45
1:C:247:GLY:O	1:C:264:LYS:NZ	2.49	0.45
1:A:46:LEU:HB3	1:A:51:MSE:HE1	1.99	0.45
1:D:180:MSE:HE3	1:D:199:ILE:CG1	2.39	0.45
1:I:43[A]:CYS:HB2	1:I:84:LYS:HA	1.98	0.45
1:D:180:MSE:HE2	1:D:197:PHE:HD1	1.81	0.45
1:N:166:PHE:CD1	1:N:166:PHE:C	2.89	0.45
1:G:230:VAL:HG12	1:G:231:ASN:OD1	2.16	0.45
1:L:196[B]:GLU:HA	1:L:216:GLU:O	2.17	0.45
1:D:72:ILE:HD12	1:D:72:ILE:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:235:ALA:O	1:E:254:LYS:HA	2.17	0.45
1:F:245:TYR:OH	1:F:252:ILE:HD13	2.16	0.45
1:G:72:ILE:CD1	1:G:101:PRO:HB3	2.47	0.45
1:H:144:ILE:HG22	1:H:146[B]:GLN:HG3	1.98	0.45
1:P:130:LEU:HD21	1:P:135:PHE:CE2	2.52	0.45
1:B:176:LEU:C	1:B:176:LEU:CD2	2.86	0.45
1:M:114:LYS:O	1:M:135:PHE:HA	2.17	0.45
1:N:65:GLU:C	1:N:66:ILE:HD12	2.36	0.45
1:P:43:CYS:HB3	1:P:115:LYS:HE2	1.98	0.45
1:D:196:GLU:HA	1:D:216:GLU:O	2.17	0.45
1:E:66:ILE:HD12	1:E:66:ILE:N	2.32	0.45
1:E:43[A]:CYS:HB2	1:E:84:LYS:HA	1.99	0.45
1:L:176:LEU:HD23	1:L:177:ASN:N	2.32	0.45
1:P:55:TYR:CG	1:P:56:THR:N	2.85	0.45
1:G:245:TYR:CZ	1:G:264:LYS:HB2	2.52	0.44
1:M:31:ILE:HD12	1:M:31:ILE:N	2.32	0.44
1:K:66:ILE:HD12	1:K:106:VAL:HG22	1.99	0.44
1:L:196[A]:GLU:HA	1:L:216:GLU:O	2.17	0.44
1:M:36:ILE:HG13	1:M:66:ILE:HD13	1.99	0.44
1:E:56:THR:HG23	2:E:283:HOH:O	2.17	0.44
1:E:176:LEU:HD23	1:E:177:ASN:N	2.33	0.44
1:M:199:ILE:HD13	1:M:203:GLY:HA3	1.99	0.44
1:F:31:ILE:HD13	1:F:69:ASP:OD1	2.17	0.44
1:G:44:LEU:HD13	1:G:85:LEU:HD23	2.00	0.44
1:I:193:GLY:O	1:I:213:ASP:HB2	2.17	0.44
1:N:68:THR:CG2	1:N:72:ILE:HG21	2.48	0.44
1:B:72:ILE:O	1:B:76:TYR:HB2	2.18	0.44
1:N:157:LYS:HE2	1:N:159:GLU:OE2	2.16	0.44
1:P:139:LEU:HD21	1:P:143:GLY:O	2.18	0.44
1:A:46:LEU:HD22	1:A:51:MSE:CE	2.48	0.44
1:O:122:THR:O	1:O:143:GLY:HA3	2.17	0.44
1:G:46:LEU:HD21	1:G:87:ILE:HD12	1.99	0.44
1:B:31:ILE:HD11	1:B:102:THR:HB	2.00	0.44
1:O:59:ASP:OD1	1:O:111[B]:ARG:NH1	2.51	0.44
1:B:180:MSE:CE	1:B:184:ASN:OD1	2.66	0.44
1:H:36:ILE:HG22	1:H:37:PRO:O	2.18	0.44
1:K:170:LYS:NZ	1:O:209:ASP:OD1	2.47	0.44
1:O:196[B]:GLU:HA	1:O:216:GLU:O	2.18	0.44
1:P:56:THR:HG23	1:P:128:SER:CB	2.42	0.44
1:E:66:ILE:HG12	1:E:78:PHE:CE2	2.53	0.43
1:G:116:LEU:CD1	1:G:124:VAL:HG11	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:247:GLY:O	1:G:264:LYS:NZ	2.48	0.43
1:K:100:ARG:NH2	1:L:261:LYS:CG	2.82	0.43
1:L:76:TYR:HA	1:L:89:PRO:HA	2.00	0.43
1:M:254:LYS:HZ1	1:N:97:THR:HG1	1.65	0.43
1:O:265:VAL:O	1:O:266:GLU:CG	2.60	0.43
1:D:59:ASP:O	1:D:111:ARG:NH1	2.52	0.43
1:H:43:CYS:HB2	1:H:84:LYS:HG2	2.00	0.43
1:M:60:ALA:HB1	1:M:61:PRO:HD2	2.00	0.43
1:A:96:HIS:O	1:A:98:ASN:N	2.38	0.43
1:B:94:ARG:O	1:B:97:THR:HG23	2.17	0.43
1:G:241:GLY:O	1:G:260:GLY:HA2	2.18	0.43
1:D:48:GLY:HA3	1:D:51:MSE:HE3	2.01	0.43
1:B:232[B]:LYS:HD3	1:B:233:ILE:N	2.33	0.43
1:I:64:LEU:HD11	1:I:66:ILE:HD11	2.01	0.43
1:D:36:ILE:HA	1:D:37:PRO:HD3	1.90	0.43
1:E:100[B]:ARG:HD3	1:E:100[B]:ARG:HA	1.56	0.43
1:F:204:THR:HG23	1:F:206:ARG:NH1	2.34	0.43
1:L:62:GLU:HG2	1:L:110:SER:HA	2.01	0.43
1:C:150:THR:HG22	1:C:170:LYS:HD3	2.00	0.43
1:D:214:GLU:HG2	1:D:232:LYS:HB3	2.01	0.43
1:O:66:ILE:HG13	1:O:78:PHE:CE2	2.54	0.43
1:P:143:GLY:O	1:P:144:ILE:HD13	2.19	0.43
1:A:245:TYR:CZ	1:A:264:LYS:HB2	2.54	0.42
1:O:116:LEU:HD23	1:O:116:LEU:C	2.40	0.42
1:A:146[A]:GLN:HA	1:A:167:VAL:O	2.19	0.42
1:A:192:VAL:O	1:A:212:MSE:HA	2.19	0.42
1:G:235:ALA:O	1:G:254:LYS:HA	2.20	0.42
1:I:97:THR:O	1:I:97:THR:CG2	2.63	0.42
1:N:96[A]:HIS:CG	1:N:97:THR:N	2.86	0.42
1:B:72:ILE:HD11	1:B:101:PRO:CG	2.42	0.42
1:I:245:TYR:CZ	1:I:264:LYS:HB2	2.54	0.42
1:K:209:ASP:CG	1:O:170:LYS:NZ	2.72	0.42
1:M:216[B]:GLU:OE1	1:M:218:LYS:NZ	2.47	0.42
1:P:66:ILE:N	1:P:66:ILE:CD1	2.80	0.42
1:A:31:ILE:HD12	1:A:31:ILE:N	2.34	0.42
1:K:245:TYR:CZ	1:K:264:LYS:HB2	2.54	0.42
1:C:224:ASP:C	1:C:224:ASP:OD1	2.58	0.42
1:E:132:ALA:O	1:E:153:PHE:HA	2.18	0.42
1:M:0:GLY:O	1:M:71:ASN:ND2	2.52	0.42
1:M:31:ILE:N	1:M:31:ILE:CD1	2.82	0.42
1:H:66:ILE:N	1:H:66:ILE:CD1	2.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:118:ALA:HB1	1:M:122:THR:HG21	2.02	0.42
1:D:265:VAL:HG13	1:F:266:GLU:HG2	2.02	0.42
1:O:196[A]:GLU:HA	1:O:216:GLU:O	2.20	0.42
1:C:245:TYR:CZ	1:C:264:LYS:HB2	2.55	0.42
1:J:96:HIS:O	1:J:97:THR:C	2.58	0.42
1:L:33:THR:CG2	1:L:34:GLU:N	2.83	0.42
1:L:116:LEU:HD21	1:L:124:VAL:HG11	2.02	0.42
1:P:146:GLN:CD	1:P:148:HIS:CE1	2.93	0.42
1:B:48:GLY:HA2	1:B:76:TYR:HH	1.84	0.42
1:L:115[B]:LYS:HE3	1:L:115[B]:LYS:HB2	1.81	0.42
1:O:254:LYS:HE3	2:O:843:HOH:O	2.19	0.42
1:B:204:THR:HG23	1:B:206:ARG:NH1	2.35	0.42
1:F:59:ASP:O	1:F:111:ARG:NH1	2.53	0.42
1:H:151:ALA:HB1	1:H:153:PHE:CZ	2.55	0.42
1:J:64:LEU:HG	1:J:66:ILE:CD1	2.50	0.42
1:J:157:LYS:CE	1:J:159:GLU:OE2	2.68	0.42
1:K:100:ARG:HA	1:K:101:PRO:HD3	1.88	0.42
1:E:100[B]:ARG:HA	1:E:101:PRO:HD3	1.81	0.41
1:F:48:GLY:CA	1:F:76:TYR:OH	2.66	0.41
1:B:232[B]:LYS:HG2	1:B:251:ASP:HB3	2.00	0.41
1:C:192:VAL:O	1:C:212:MSE:HA	2.19	0.41
1:N:66:ILE:HG22	1:N:73:PHE:CZ	2.56	0.41
1:O:96:HIS:O	1:O:98:ASN:N	2.53	0.41
1:C:258:GLY:HA2	1:D:47:GLU:HG3	2.02	0.41
1:E:166:PHE:CD1	1:E:166:PHE:C	2.93	0.41
1:J:176:LEU:HD23	1:J:177:ASN:N	2.35	0.41
1:L:233:ILE:HG23	1:L:252:ILE:HG23	2.01	0.41
1:D:98:ASN:O	1:D:99:PHE:CB	2.69	0.41
1:G:46:LEU:HD23	1:G:87:ILE:HD12	2.03	0.41
1:G:51:MSE:HG2	1:G:104:PHE:CD1	2.55	0.41
1:B:56:THR:HG23	2:B:267:HOH:O	2.20	0.41
1:G:123:HIS:ND1	2:G:270:HOH:O	2.37	0.41
1:I:207:ALA:HB1	1:I:212:MSE:HE3	2.03	0.41
1:E:114:LYS:O	1:E:135:PHE:HA	2.21	0.41
1:O:235:ALA:O	1:O:254:LYS:HA	2.20	0.41
1:P:160:ILE:HG22	1:P:184:ASN:HD22	1.85	0.41
1:A:139:LEU:HD23	1:A:164:GLY:HA3	2.02	0.41
1:D:176:LEU:C	1:D:176:LEU:CD2	2.88	0.41
1:O:265:VAL:O	1:O:266:GLU:CB	2.68	0.41
1:A:192:VAL:HG23	1:A:210:CYS:SG	2.61	0.41
1:C:186:ILE:HG22	1:C:188:LEU:HG	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:165:ASP:OD1	1:J:185:THR:HB	2.20	0.41
1:N:64:LEU:HG	1:N:66:ILE:CD1	2.51	0.41
1:D:153:PHE:O	1:D:173:CYS:HA	2.21	0.41
1:H:64:LEU:HG	1:H:66:ILE:HD11	2.02	0.41
1:H:153:PHE:O	1:H:173:CYS:HA	2.20	0.41
1:M:126:ILE:HG13	1:M:147:PHE:CE1	2.55	0.41
1:P:146:GLN:HG3	1:P:167:VAL:HB	2.03	0.41
1:A:131:GLN:NE2	2:A:668:HOH:O	2.54	0.41
1:M:43[A]:CYS:HB2	1:M:84:LYS:HA	2.03	0.41
1:H:65:GLU:C	1:H:66:ILE:HD12	2.41	0.40
1:K:32:THR:HG21	1:K:34:GLU:OE2	2.21	0.40
1:N:43:CYS:HB2	1:N:84:LYS:HG2	2.03	0.40
1:M:216[B]:GLU:OE2	1:M:234:LYS:NZ	2.47	0.40
1:A:146[B]:GLN:HA	1:A:167:VAL:O	2.21	0.40
1:N:68:THR:CG2	1:N:72:ILE:HG23	2.50	0.40
1:O:55:TYR:CZ	1:O:113:LEU:HD22	2.57	0.40
1:A:46:LEU:HD23	1:A:51:MSE:CE	2.35	0.40
1:B:232[B]:LYS:HE3	1:B:234:LYS:HB2	2.03	0.40
1:I:66:ILE:N	1:I:66:ILE:CD1	2.84	0.40
1:I:114:LYS:O	1:I:135:PHE:HA	2.22	0.40
1:I:139:LEU:HD22	1:I:145:ILE:HG13	2.02	0.40
1:J:43:CYS:HB2	1:J:84:LYS:HG2	2.03	0.40
1:O:151:ALA:HB1	1:O:153:PHE:CZ	2.57	0.40
1:A:47[B]:GLU:HG2	1:A:119:ALA:HB3	2.03	0.40
1:A:96:HIS:HA	1:B:255:LYS:NZ	2.37	0.40
1:C:170:LYS:NZ	1:G:209:ASP:OD1	2.33	0.40
1:P:235:ALA:HB3	1:P:262:ILE:HD13	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	246/241 (102%)	236 (96%)	8 (3%)	2 (1%)	19	23
1	B	238/241 (99%)	224 (94%)	14 (6%)	0	100	100
1	C	247/241 (102%)	232 (94%)	15 (6%)	0	100	100
1	D	240/241 (100%)	231 (96%)	9 (4%)	0	100	100
1	E	244/241 (101%)	236 (97%)	8 (3%)	0	100	100
1	F	241/241 (100%)	231 (96%)	10 (4%)	0	100	100
1	G	244/241 (101%)	232 (95%)	12 (5%)	0	100	100
1	H	245/241 (102%)	234 (96%)	11 (4%)	0	100	100
1	I	244/241 (101%)	234 (96%)	10 (4%)	0	100	100
1	J	241/241 (100%)	231 (96%)	10 (4%)	0	100	100
1	K	244/241 (101%)	237 (97%)	7 (3%)	0	100	100
1	L	237/241 (98%)	223 (94%)	14 (6%)	0	100	100
1	M	249/241 (103%)	237 (95%)	12 (5%)	0	100	100
1	N	243/241 (101%)	231 (95%)	12 (5%)	0	100	100
1	O	243/241 (101%)	233 (96%)	10 (4%)	0	100	100
1	P	229/241 (95%)	216 (94%)	13 (6%)	0	100	100
All	All	3875/3856 (100%)	3698 (95%)	175 (4%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	97	THR

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	194/190 (102%)	194 (100%)	0	100	100
1	B	186/190 (98%)	185 (100%)	1 (0%)	88	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	193/190 (102%)	192 (100%)	1 (0%)	88	95
1	D	181/190 (95%)	179 (99%)	2 (1%)	73	86
1	E	194/190 (102%)	193 (100%)	1 (0%)	88	95
1	F	184/190 (97%)	183 (100%)	1 (0%)	88	95
1	G	188/190 (99%)	187 (100%)	1 (0%)	88	95
1	H	188/190 (99%)	186 (99%)	2 (1%)	73	86
1	I	190/190 (100%)	190 (100%)	0	100	100
1	J	190/190 (100%)	188 (99%)	2 (1%)	73	86
1	K	192/190 (101%)	191 (100%)	1 (0%)	88	95
1	L	180/190 (95%)	178 (99%)	2 (1%)	73	86
1	M	200/190 (105%)	200 (100%)	0	100	100
1	N	194/190 (102%)	192 (99%)	2 (1%)	76	87
1	O	195/190 (103%)	195 (100%)	0	100	100
1	P	167/190 (88%)	166 (99%)	1 (1%)	86	94
All	All	3016/3040 (99%)	2999 (99%)	17 (1%)	86	94

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	104	PHE
1	C	104	PHE
1	D	69	ASP
1	D	104	PHE
1	E	104	PHE
1	F	104	PHE
1	G	69	ASP
1	H	104	PHE
1	H	109	ASN
1	J	104	PHE
1	J	174	GLU
1	K	104	PHE
1	L	93	PHE
1	L	104	PHE
1	N	104	PHE
1	N	174	GLU
1	P	104	PHE

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

Mol	Chain	Res	Type
1	D	253	GLN
1	H	109	ASN
1	J	83	HIS

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, 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	236/241 (97%)	0.50	3 (1%) 77 81	22, 32, 44, 64	0
1	B	232/241 (96%)	1.04	41 (17%) 1 1	30, 42, 53, 72	0
1	C	236/241 (97%)	0.36	4 (1%) 70 76	24, 33, 44, 63	0
1	D	235/241 (97%)	0.93	37 (15%) 2 2	29, 42, 52, 69	0
1	E	236/241 (97%)	0.51	8 (3%) 45 52	23, 32, 45, 64	0
1	F	234/241 (97%)	1.05	40 (17%) 1 2	29, 42, 54, 68	0
1	G	236/241 (97%)	0.37	5 (2%) 63 70	24, 33, 44, 63	0
1	H	236/241 (97%)	0.81	28 (11%) 4 6	30, 42, 55, 65	0
1	I	236/241 (97%)	0.50	9 (3%) 40 47	23, 32, 44, 64	0
1	J	233/241 (96%)	1.10	40 (17%) 1 1	29, 42, 52, 64	0
1	K	236/241 (97%)	0.30	4 (1%) 70 76	23, 33, 44, 60	0
1	L	230/241 (95%)	0.92	30 (13%) 3 4	30, 42, 50, 62	0
1	M	236/241 (97%)	0.56	11 (4%) 31 38	23, 32, 44, 62	0
1	N	233/241 (96%)	1.02	38 (16%) 1 2	29, 42, 52, 64	0
1	O	235/241 (97%)	0.34	3 (1%) 77 81	24, 33, 44, 60	0
1	P	227/241 (94%)	1.03	35 (15%) 2 3	30, 42, 49, 60	0
All	All	3747/3856 (97%)	0.71	336 (8%) 9 12	22, 37, 50, 72	0

All (336) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	102	THR	8.8
1	D	0	GLY	7.8
1	H	98	ASN	7.1
1	P	93	PHE	6.8
1	L	93	PHE	6.6

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Mol	Chain	Res	Type	RSRZ
1	D	99	PHE	6.6
1	D	98	ASN	6.5
1	B	98	ASN	6.3
1	F	66	ILE	6.1
1	F	28	ASP	6.1
1	F	29	GLY	6.1
1	N	96[A]	HIS	6.0
1	H	97	THR	5.8
1	P	73	PHE	5.7
1	N	72	ILE	5.7
1	J	28	ASP	5.7
1	D	27	GLY	5.7
1	J	99	PHE	5.6
1	I	100	ARG	5.6
1	G	96	HIS	5.6
1	E	96	HIS	5.5
1	P	61	PRO	5.5
1	J	60	ALA	5.5
1	P	64	LEU	5.5
1	B	66	ILE	5.4
1	J	92	GLU	5.4
1	N	99	PHE	5.4
1	D	50	GLY	5.3
1	N	102	THR	5.3
1	J	93	PHE	5.3
1	L	49	GLY	5.3
1	P	33	THR	5.3
1	B	99	PHE	5.3
1	D	102	THR	5.3
1	H	28	ASP	5.3
1	N	97	THR	5.3
1	L	27	GLY	5.3
1	P	49	GLY	5.2
1	J	32	THR	5.2
1	L	28	ASP	5.2
1	M	97	THR	5.1
1	P	76	TYR	5.1
1	J	98	ASN	5.0
1	J	97	THR	5.0
1	P	70	ARG	4.9
1	D	100	ARG	4.9
1	K	97	THR	4.9

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Mol	Chain	Res	Type	RSRZ
1	F	30	ASN	4.8
1	A	97	THR	4.7
1	F	55	TYR	4.7
1	B	72	ILE	4.7
1	H	0	GLY	4.7
1	M	99[A]	PHE	4.6
1	L	90	LYS	4.6
1	B	35	ASN	4.6
1	F	96	HIS	4.5
1	N	32	THR	4.5
1	H	27	GLY	4.5
1	O	266	GLU	4.5
1	N	101	PRO	4.4
1	G	0	GLY	4.4
1	B	108	ALA	4.4
1	J	102	THR	4.4
1	A	96	HIS	4.4
1	H	96	HIS	4.4
1	N	91	LYS	4.4
1	J	30	ASN	4.4
1	J	61	PRO	4.3
1	P	35	ASN	4.3
1	N	100	ARG	4.3
1	F	108	ALA	4.3
1	N	76	TYR	4.3
1	J	107	THR	4.3
1	N	31	ILE	4.3
1	D	72	ILE	4.2
1	P	72	ILE	4.2
1	B	100	ARG	4.2
1	P	104	PHE	4.2
1	P	38	VAL	4.1
1	H	29	GLY	4.1
1	B	95	LYS	4.1
1	D	95	LYS	4.1
1	F	99	PHE	4.1
1	F	32	THR	4.1
1	J	33	THR	4.0
1	H	73	PHE	4.0
1	M	96	HIS	4.0
1	L	72	ILE	3.9
1	J	31	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	28	ASP	3.9
1	N	92	GLU	3.9
1	J	76	TYR	3.9
1	L	61	PRO	3.9
1	H	71	ASN	3.9
1	N	98	ASN	3.9
1	F	64	LEU	3.8
1	B	96	HIS	3.8
1	F	97	THR	3.7
1	P	66	ILE	3.7
1	L	101	PRO	3.7
1	D	71	ASN	3.7
1	L	35	ASN	3.7
1	F	72	ILE	3.7
1	F	171	VAL	3.7
1	E	266	GLU	3.6
1	P	74	GLU	3.6
1	N	73	PHE	3.5
1	D	36	ILE	3.5
1	B	59	ASP	3.5
1	N	60	ALA	3.5
1	F	36	ILE	3.5
1	N	61	PRO	3.5
1	B	68	THR	3.5
1	D	29	GLY	3.5
1	N	30	ASN	3.4
1	F	95	LYS	3.4
1	B	101	PRO	3.4
1	F	63	GLY	3.4
1	P	41	TYR	3.4
1	B	31	ILE	3.4
1	F	98	ASN	3.4
1	M	100	ARG	3.4
1	D	61	PRO	3.4
1	B	34	GLU	3.4
1	C	97	THR	3.3
1	L	70	ARG	3.3
1	B	97	THR	3.3
1	B	36	ILE	3.3
1	F	126	ILE	3.3
1	P	68	THR	3.3
1	N	59	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	97	THR	3.3
1	M	72	ILE	3.2
1	D	60	ALA	3.2
1	C	266	GLU	3.2
1	J	72	ILE	3.2
1	L	74	GLU	3.2
1	P	90	LYS	3.2
1	C	96	HIS	3.1
1	F	128	SER	3.1
1	I	266	GLU	3.1
1	B	64	LEU	3.1
1	J	38	VAL	3.1
1	N	129	PRO	3.1
1	J	65	GLU	3.1
1	H	133[A]	GLU	3.1
1	P	36	ILE	3.1
1	D	78	PHE	3.1
1	I	96	HIS	3.1
1	J	59	ASP	3.1
1	P	69	ASP	3.1
1	F	109	ASN	3.1
1	N	65	GLU	3.1
1	B	63	GLY	3.0
1	D	49	GLY	3.0
1	F	50	GLY	3.0
1	D	96	HIS	3.0
1	E	99	PHE	3.0
1	M	0	GLY	3.0
1	B	55	TYR	3.0
1	H	59	ASP	3.0
1	L	65	GLU	3.0
1	P	59	ASP	3.0
1	E	100[A]	ARG	3.0
1	B	92	GLU	3.0
1	B	38	VAL	3.0
1	J	73	PHE	3.0
1	P	65	GLU	2.9
1	P	124	VAL	2.9
1	G	97	THR	2.9
1	H	63	GLY	2.9
1	J	46	LEU	2.9
1	L	76	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	35	ASN	2.9
1	P	63	GLY	2.9
1	P	40	GLU	2.9
1	H	99	PHE	2.9
1	B	110	SER	2.9
1	N	39	SER	2.9
1	J	109	ASN	2.9
1	B	60	ALA	2.9
1	F	110	SER	2.8
1	D	93	PHE	2.8
1	N	93	PHE	2.8
1	N	103	GLU	2.8
1	J	37	PRO	2.8
1	P	101	PRO	2.8
1	P	92	GLU	2.8
1	J	100	ARG	2.8
1	N	48	GLY	2.8
1	L	38	VAL	2.8
1	N	37	PRO	2.8
1	B	94	ARG	2.8
1	F	59	ASP	2.8
1	F	34[A]	GLU	2.8
1	F	101	PRO	2.8
1	N	71	ASN	2.8
1	D	31	ILE	2.8
1	M	31	ILE	2.8
1	E	260	GLY	2.8
1	P	102	THR	2.8
1	L	66	ILE	2.7
1	B	91	LYS	2.7
1	P	71	ASN	2.7
1	F	104	PHE	2.7
1	N	38	VAL	2.7
1	J	44	LEU	2.7
1	D	65	GLU	2.7
1	B	93	PHE	2.7
1	F	92	GLU	2.7
1	H	38	VAL	2.7
1	J	48	GLY	2.7
1	P	31	ILE	2.6
1	C	99	PHE	2.6
1	H	40	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	92[A]	GLU	2.6
1	P	60	ALA	2.6
1	I	93	PHE	2.6
1	L	127	ASN	2.6
1	F	100	ARG	2.6
1	B	130	LEU	2.6
1	D	66	ILE	2.6
1	P	107	THR	2.6
1	N	94	ARG	2.6
1	H	101	PRO	2.5
1	H	50	GLY	2.5
1	D	266	GLU	2.5
1	H	72	ILE	2.5
1	J	50	GLY	2.5
1	L	39	SER	2.5
1	K	99	PHE	2.5
1	B	71	ASN	2.5
1	B	189	GLY	2.5
1	I	72	ILE	2.5
1	J	29	GLY	2.5
1	K	96	HIS	2.4
1	G	266	GLU	2.4
1	H	60	ALA	2.4
1	I	98	ASN	2.4
1	H	61	PRO	2.4
1	H	48	GLY	2.4
1	D	41	TYR	2.4
1	H	62	GLU	2.4
1	L	112[A]	ASN	2.4
1	F	60	ALA	2.4
1	D	73	PHE	2.4
1	P	83	HIS	2.4
1	M	102	THR	2.4
1	N	35	ASN	2.4
1	M	94	ARG	2.4
1	D	38	VAL	2.4
1	P	127	ASN	2.4
1	J	96	HIS	2.4
1	L	75	LYS	2.3
1	F	37	PRO	2.3
1	J	103	GLU	2.3
1	F	80	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	75	LYS	2.3
1	L	64	LEU	2.3
1	J	78	PHE	2.3
1	N	90	LYS	2.3
1	B	89	PRO	2.3
1	F	71	ASN	2.3
1	J	152	SER	2.3
1	B	50	GLY	2.3
1	L	78	PHE	2.3
1	D	79	ASN	2.3
1	B	40	GLU	2.3
1	J	128	SER	2.3
1	N	111[A]	ARG	2.3
1	J	140	ALA	2.3
1	P	48	GLY	2.3
1	L	71	ASN	2.3
1	N	109	ASN	2.3
1	F	68	THR	2.2
1	F	102	THR	2.2
1	F	43	CYS	2.2
1	H	127	ASN	2.2
1	B	153	PHE	2.2
1	I	99	PHE	2.2
1	J	39	SER	2.2
1	D	69	ASP	2.2
1	B	104	PHE	2.2
1	D	128	SER	2.2
1	B	79	ASN	2.2
1	N	131	GLN	2.2
1	F	61	PRO	2.2
1	P	106	VAL	2.2
1	H	35	ASN	2.2
1	J	68	THR	2.2
1	N	44	LEU	2.2
1	D	126	ILE	2.2
1	L	31	ILE	2.2
1	B	37	PRO	2.2
1	D	92[A]	GLU	2.2
1	K	266	GLU	2.2
1	O	99	PHE	2.2
1	O	103	GLU	2.2
1	B	132	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	32	THR	2.1
1	L	43	CYS	2.1
1	F	112	ASN	2.1
1	M	123	HIS	2.1
1	H	266	GLU	2.1
1	F	69	ASP	2.1
1	B	109	ASN	2.1
1	H	37	PRO	2.1
1	F	111	ARG	2.1
1	D	33	THR	2.1
1	L	68	THR	2.1
1	B	112	ASN	2.1
1	D	48	GLY	2.1
1	J	198[A]	SER	2.1
1	E	91	LYS	2.1
1	L	73	PHE	2.1
1	E	101	PRO	2.1
1	N	139	LEU	2.1
1	N	69	ASP	2.1
1	H	36	ILE	2.1
1	L	69	ASP	2.0
1	D	127	ASN	2.0
1	J	35	ASN	2.0
1	A	140	ALA	2.0
1	I	140	ALA	2.0
1	L	29	GLY	2.0
1	J	129	PRO	2.0
1	L	106	VAL	2.0
1	N	36	ILE	2.0
1	F	155	ASN	2.0
1	I	27	GLY	2.0
1	J	142[A]	SER	2.0
1	B	171	VAL	2.0
1	G	46	LEU	2.0
1	M	266	GLU	2.0
1	D	248	ASP	2.0
1	N	33	THR	2.0

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

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.