



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:56 PM UTC

PDB ID : 8RKZ / pdb_00008rkz
Title : Crystal structure of a cysteine hydrolase from *Phytophthora infestans*
Authors : Altegoer, F.; Weiland, P.; Bange, G.
Deposited on : 2024-01-02
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

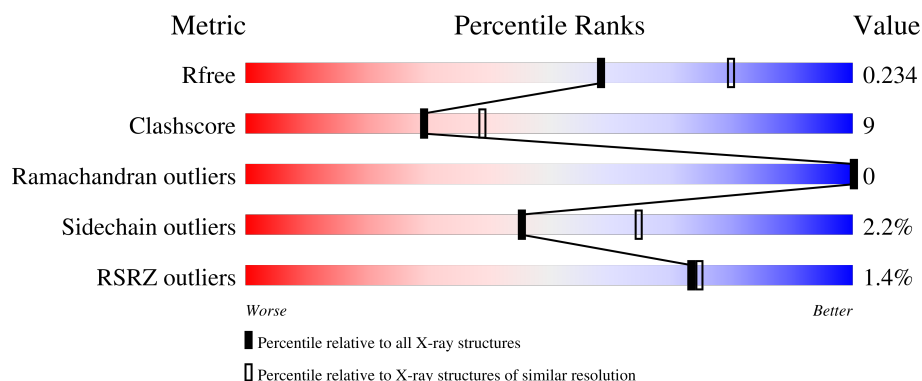
1 Overall quality at a glance

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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	209	2% 77% 20% •
1	B	209	2% 79% 15% • 5%
1	C	209	71% 22% • 5%
1	D	209	2% 78% 17% 5%
1	E	209	75% 20% 5%

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Mol	Chain	Length	Quality of chain
1	F	209	 2% 77% 18% 5%
1	G	209	 3% 75% 19% • 5%
1	H	209	 % 81% 13% 5%
1	I	209	 78% 16% 5%
1	J	209	 78% 15% • 5%
1	K	209	 2% 77% 16% • 6%
1	L	209	 % 79% 15% 5%
1	M	209	 2% 81% 13% • 5%
1	N	209	 % 75% 19% • 5%
1	O	209	 2% 76% 19% 5%
1	P	209	 2% 64% 30% • 5%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 25784 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 Isochorismatase family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	198	Total	C	N	O	S	0	0	0
			1530	967	260	293	10			
1	H	198	Total	C	N	O	S	0	0	0
			1536	970	263	293	10			
1	L	198	Total	C	N	O	S	0	1	0
			1542	973	264	294	11			
1	M	198	Total	C	N	O	S	0	1	0
			1542	973	264	294	11			
1	D	198	Total	C	N	O	S	0	0	0
			1536	970	263	293	10			
1	J	198	Total	C	N	O	S	0	0	0
			1536	970	263	293	10			
1	I	198	Total	C	N	O	S	0	0	0
			1536	970	263	293	10			
1	K	196	Total	C	N	O	S	0	0	0
			1521	961	260	290	10			
1	A	201	Total	C	N	O	S	0	0	0
			1547	978	263	296	10			
1	P	198	Total	C	N	O	S	0	1	0
			1529	964	260	294	11			
1	O	198	Total	C	N	O	S	0	1	0
			1542	973	264	294	11			
1	N	198	Total	C	N	O	S	0	1	0
			1542	973	264	294	11			
1	B	198	Total	C	N	O	S	0	0	0
			1536	970	263	293	10			
1	C	198	Total	C	N	O	S	0	0	0
			1536	970	263	293	10			
1	F	198	Total	C	N	O	S	0	0	0
			1536	970	263	293	10			
1	E	198	Total	C	N	O	S	0	0	0
			1536	970	263	293	10			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	2	GLY	ALA	conflict	UNP A0A833SVL6
G	197	LEU	ARG	conflict	UNP A0A833SVL6
H	2	GLY	ALA	conflict	UNP A0A833SVL6
H	197	LEU	ARG	conflict	UNP A0A833SVL6
L	2	GLY	ALA	conflict	UNP A0A833SVL6
L	197	LEU	ARG	conflict	UNP A0A833SVL6
M	2	GLY	ALA	conflict	UNP A0A833SVL6
M	197	LEU	ARG	conflict	UNP A0A833SVL6
D	2	GLY	ALA	conflict	UNP A0A833SVL6
D	197	LEU	ARG	conflict	UNP A0A833SVL6
J	2	GLY	ALA	conflict	UNP A0A833SVL6
J	197	LEU	ARG	conflict	UNP A0A833SVL6
I	2	GLY	ALA	conflict	UNP A0A833SVL6
I	197	LEU	ARG	conflict	UNP A0A833SVL6
K	2	GLY	ALA	conflict	UNP A0A833SVL6
K	197	LEU	ARG	conflict	UNP A0A833SVL6
A	2	GLY	ALA	conflict	UNP A0A833SVL6
A	197	LEU	ARG	conflict	UNP A0A833SVL6
P	2	GLY	ALA	conflict	UNP A0A833SVL6
P	197	LEU	ARG	conflict	UNP A0A833SVL6
O	2	GLY	ALA	conflict	UNP A0A833SVL6
O	197	LEU	ARG	conflict	UNP A0A833SVL6
N	2	GLY	ALA	conflict	UNP A0A833SVL6
N	197	LEU	ARG	conflict	UNP A0A833SVL6
B	2	GLY	ALA	conflict	UNP A0A833SVL6
B	197	LEU	ARG	conflict	UNP A0A833SVL6
C	2	GLY	ALA	conflict	UNP A0A833SVL6
C	197	LEU	ARG	conflict	UNP A0A833SVL6
F	2	GLY	ALA	conflict	UNP A0A833SVL6
F	197	LEU	ARG	conflict	UNP A0A833SVL6
E	2	GLY	ALA	conflict	UNP A0A833SVL6
E	197	LEU	ARG	conflict	UNP A0A833SVL6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	54	Total O 54 54	0	0
2	H	60	Total O 60 60	0	0
2	L	68	Total O 68 68	0	0

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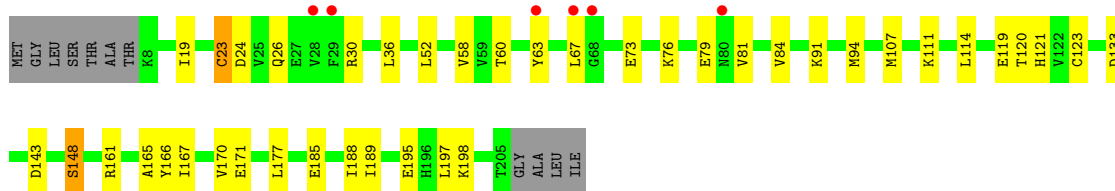
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	M	79	Total	O	0	0
			79	79		
2	D	88	Total	O	0	0
			88	88		
2	J	93	Total	O	0	0
			93	93		
2	I	89	Total	O	0	0
			89	89		
2	K	101	Total	O	0	0
			101	101		
2	A	89	Total	O	0	0
			89	89		
2	P	62	Total	O	0	0
			62	62		
2	O	63	Total	O	0	0
			63	63		
2	N	70	Total	O	0	0
			70	70		
2	B	91	Total	O	0	0
			91	91		
2	C	66	Total	O	0	0
			66	66		
2	F	60	Total	O	0	0
			60	60		
2	E	68	Total	O	0	0
			68	68		

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.

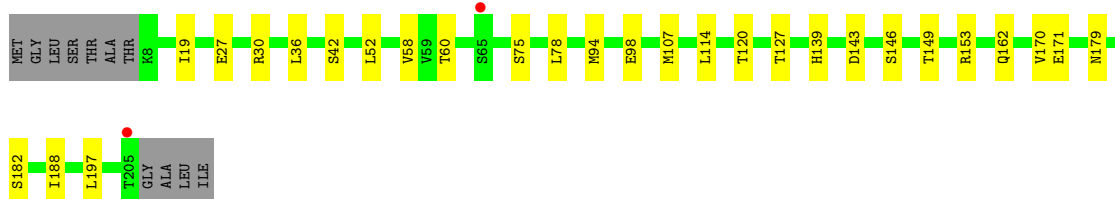
- Molecule 1: Isochorismatase family

Chain G: 



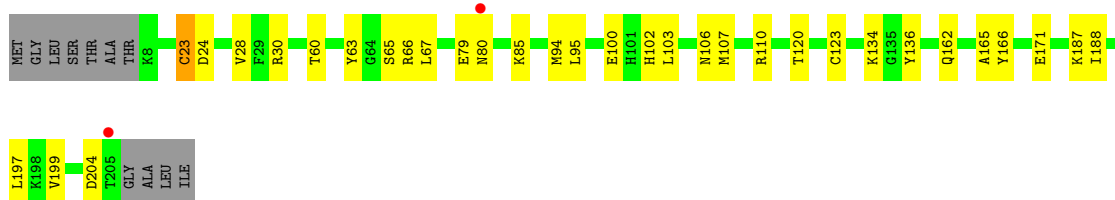
- Molecule 1: Isochorismatase family

Chain H: 



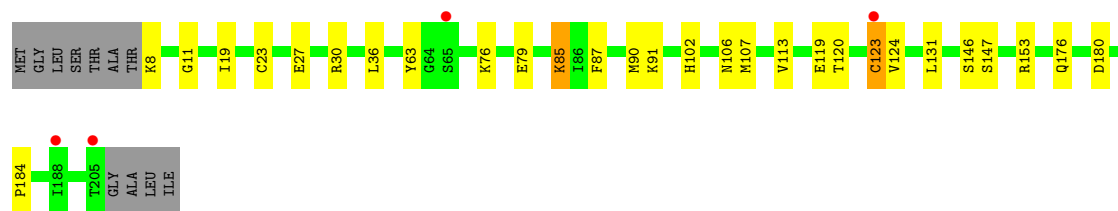
- Molecule 1: Isochorismatase family

Chain L: 

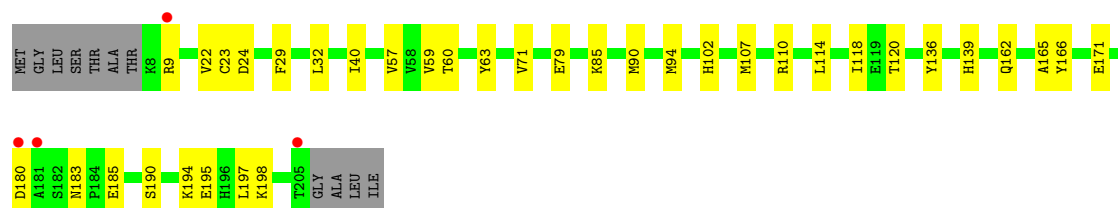
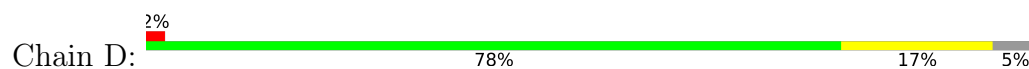


- Molecule 1: Isochorismatase family

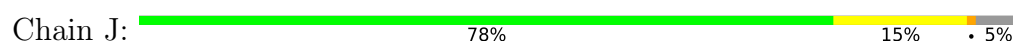
Chain M: 



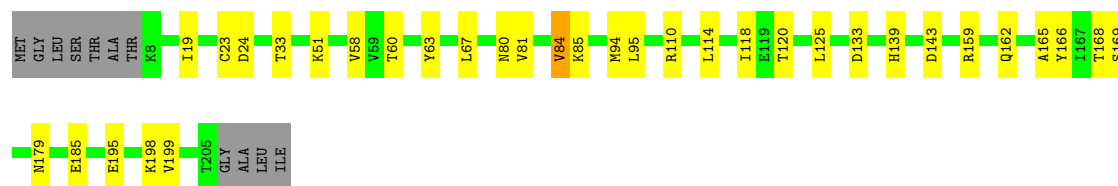
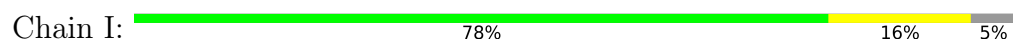
- Molecule 1: Isochorismatase family



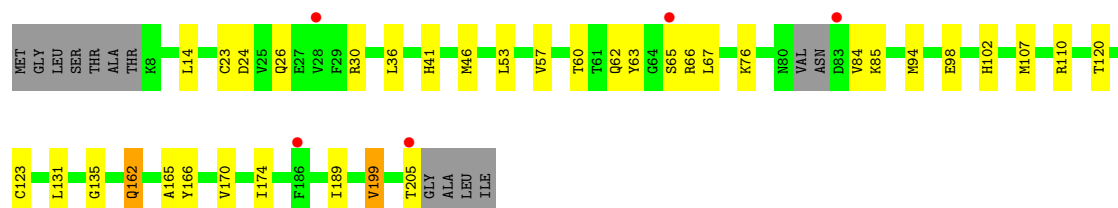
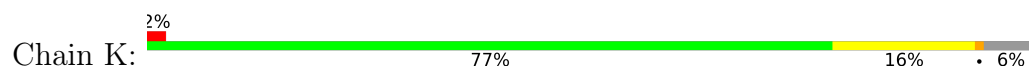
- Molecule 1: Isochorismatase family



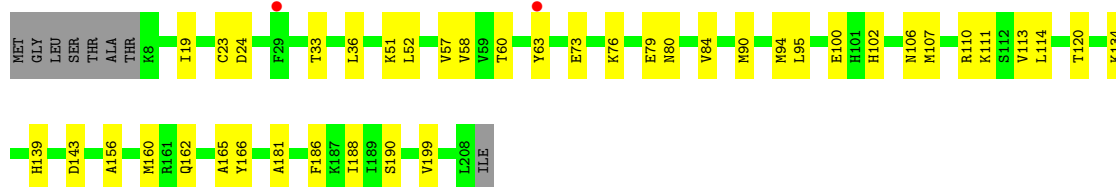
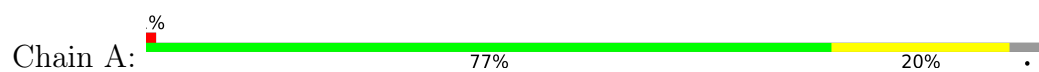
- Molecule 1: Isochorismatase family



- Molecule 1: Isochorismatase family



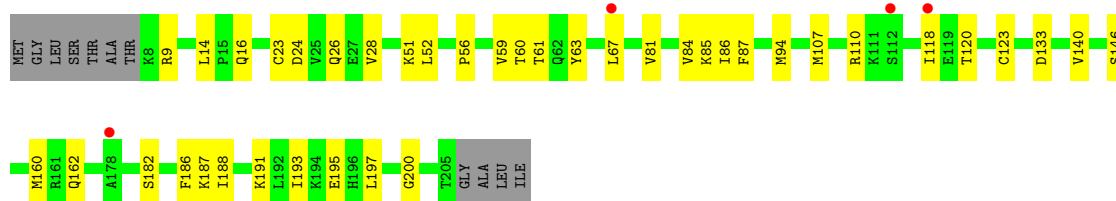
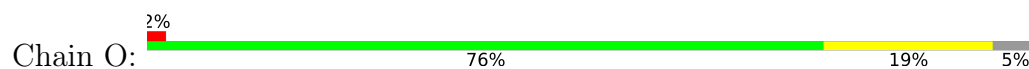
- Molecule 1: Isochorismatase family



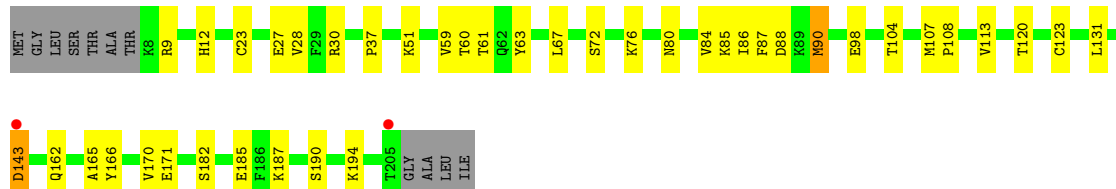
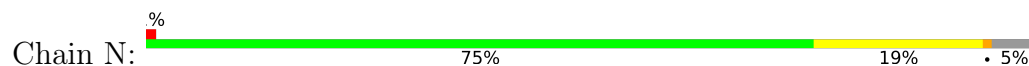
- Molecule 1: Isochorismatase family



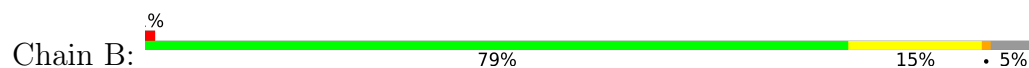
- Molecule 1: Isochorismatase family

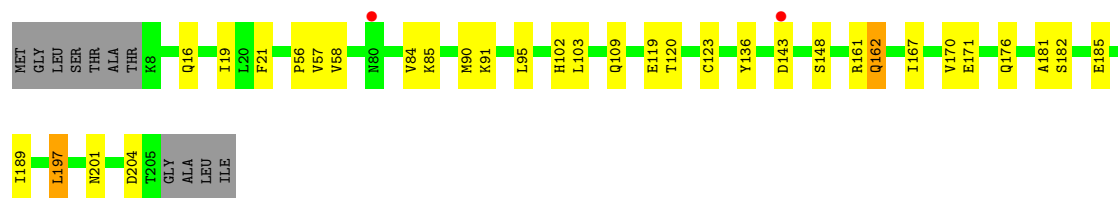


- Molecule 1: Isochorismatase family



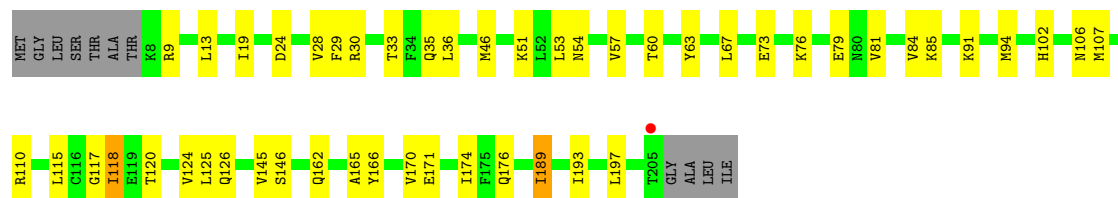
- Molecule 1: Isochorismatase family





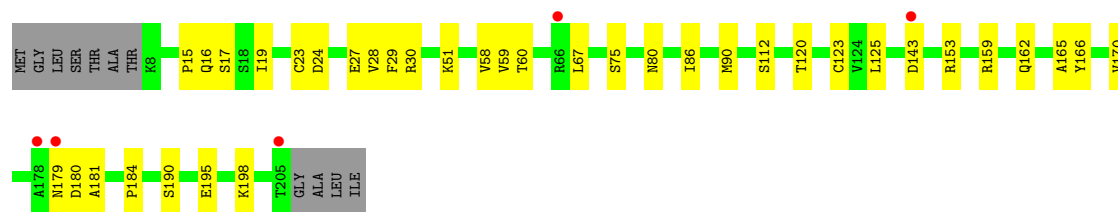
- Molecule 1: Isochorismatase family

Chain C: 71% 22% 5%



- Molecule 1: Isochorismatase family

Chain F: 77% 18% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.34Å 218.35Å 101.59Å 90.00° 102.41° 90.00°	Depositor
Resolution (Å)	47.83 – 2.30 47.83 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.83-2.30) 89.4 (47.83-2.30)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.70 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.191 , 0.235 0.191 , 0.234	Depositor DCC
R_{free} test set	7632 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25784	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.18	0/1571	0.39	0/2127
1	B	0.19	0/1560	0.38	0/2111
1	C	0.20	0/1560	0.40	0/2111
1	D	0.18	0/1560	0.40	0/2111
1	E	0.17	0/1560	0.39	2/2111 (0.1%)
1	F	0.16	0/1560	0.35	0/2111
1	G	0.18	0/1554	0.37	0/2104
1	H	0.16	0/1560	0.34	0/2111
1	I	0.17	0/1560	0.35	0/2111
1	J	0.17	0/1560	0.39	0/2111
1	K	0.19	0/1544	0.40	0/2087
1	L	0.17	0/1566	0.40	0/2119
1	M	0.16	0/1566	0.37	0/2119
1	N	0.16	0/1566	0.36	0/2119
1	O	0.17	0/1566	0.37	0/2119
1	P	0.17	0/1553	0.39	0/2104
All	All	0.17	0/24966	0.38	2/33786 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	118	ILE	CA-C-N	5.22	131.10	121.70
1	E	118	ILE	C-N-CA	5.22	131.10	121.70

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	1547	0	1576	32	0
1	B	1536	0	1568	28	0
1	C	1536	0	1568	33	0
1	D	1536	0	1568	26	0
1	E	1536	0	1568	31	0
1	F	1536	0	1568	27	0
1	G	1530	0	1555	28	0
1	H	1536	0	1568	21	0
1	I	1536	0	1568	26	0
1	J	1536	0	1568	28	0
1	K	1521	0	1552	29	0
1	L	1542	0	1570	30	0
1	M	1542	0	1570	21	0
1	N	1542	0	1570	30	0
1	O	1542	0	1570	33	0
1	P	1529	0	1539	54	0
2	A	89	0	0	2	0
2	B	91	0	0	5	0
2	C	66	0	0	7	0
2	D	88	0	0	4	0
2	E	68	0	0	3	0
2	F	60	0	0	4	0
2	G	54	0	0	1	0
2	H	60	0	0	1	0
2	I	89	0	0	5	0
2	J	93	0	0	9	0
2	K	101	0	0	6	0
2	L	68	0	0	2	0
2	M	79	0	0	5	0
2	N	70	0	0	7	0
2	O	63	0	0	1	0
2	P	62	0	0	9	0
All	All	25784	0	25046	425	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 9.

All (425) 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:O:200:GLY:O	2:O:301:HOH:O	1.83	0.95
1:L:136:TYR:O	2:L:301:HOH:O	1.86	0.94
1:P:136:TYR:O	2:P:301:HOH:O	1.87	0.92
1:J:91:LYS:NZ	2:J:303:HOH:O	2.06	0.89
1:A:73:GLU:OE2	2:A:301:HOH:O	1.91	0.85
1:F:184:PRO:O	2:F:301:HOH:O	1.95	0.84
1:P:158:GLU:OE2	2:P:302:HOH:O	1.95	0.84
1:N:87:PHE:HE2	1:N:98:GLU:HG2	1.44	0.82
1:I:110:ARG:NH1	2:I:302:HOH:O	2.12	0.82
1:P:180:ASP:OD2	2:P:303:HOH:O	1.97	0.81
1:M:11:GLY:O	2:M:301:HOH:O	1.99	0.81
1:N:113:VAL:HG11	1:N:131:LEU:HD13	1.63	0.81
1:K:26:GLN:HE22	1:K:62:GLN:H	1.28	0.81
1:I:85:LYS:NZ	2:I:303:HOH:O	2.13	0.80
1:F:179:ASN:OD1	2:F:302:HOH:O	1.99	0.80
1:M:176:GLN:NE2	2:M:301:HOH:O	2.15	0.80
1:J:171:GLU:OE1	2:J:301:HOH:O	2.02	0.78
1:N:185:GLU:N	1:N:185:GLU:OE2	2.14	0.78
1:G:52:LEU:HD23	1:G:189:ILE:HD13	1.67	0.77
1:J:88:ASP:OD2	2:J:302:HOH:O	2.03	0.77
1:D:136:TYR:O	2:D:301:HOH:O	2.02	0.76
1:B:167:ILE:H	1:E:162:GLN:HE22	1.32	0.76
1:C:30:ARG:NH2	2:C:303:HOH:O	2.18	0.76
1:N:171:GLU:OE1	2:N:301:HOH:O	2.04	0.75
1:P:54:ASN:O	2:P:304:HOH:O	2.04	0.74
1:A:90:MET:HG2	1:N:182:SER:HB3	1.68	0.74
1:C:54:ASN:ND2	2:C:305:HOH:O	2.19	0.74
1:P:123[A]:CYS:SG	2:P:353:HOH:O	2.46	0.73
1:K:53:LEU:HD21	1:K:189:ILE:HD11	1.71	0.73
1:J:61:THR:OG1	2:J:304:HOH:O	2.06	0.73
1:N:171:GLU:OE2	2:N:302:HOH:O	2.07	0.72
1:E:182:SER:O	2:E:301:HOH:O	2.06	0.72
1:J:165:ALA:O	1:I:162:GLN:NE2	2.21	0.72
1:K:107:MET:HB2	1:K:110:ARG:HG3	1.71	0.71
1:C:35:GLN:OE1	2:C:301:HOH:O	2.08	0.71
1:K:135:GLY:O	2:K:301:HOH:O	2.07	0.70
1:L:28:VAL:HG11	1:L:67:LEU:HD12	1.73	0.70
1:H:27:GLU:OE2	1:H:30:ARG:NH2	2.24	0.70
1:O:52:LEU:HD13	1:O:188:ILE:HG13	1.72	0.69
1:K:60:THR:HG21	1:K:94:MET:HG2	1.75	0.69
1:A:107:MET:HB2	1:A:110:ARG:HG3	1.76	0.68
1:K:26:GLN:NE2	1:K:62:GLN:H	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:GLN:NE2	1:K:165:ALA:O	2.25	0.67
1:D:107:MET:HB2	1:D:110:ARG:HG3	1.76	0.67
1:A:63:TYR:CD1	1:A:90:MET:HE1	2.30	0.67
1:A:24:ASP:OD1	1:A:60:THR:HG23	1.95	0.67
1:G:143:ASP:OD2	2:G:301:HOH:O	2.12	0.67
1:I:95:LEU:O	2:I:301:HOH:O	2.12	0.67
1:C:171:GLU:OE1	2:C:302:HOH:O	2.13	0.67
1:I:179:ASN:OD1	2:I:304:HOH:O	2.13	0.66
1:N:28:VAL:HG11	1:N:67:LEU:HB3	1.77	0.66
1:L:103:LEU:HD23	1:L:107:MET:HE3	1.78	0.66
1:C:46:MET:HE3	1:C:170:VAL:HA	1.78	0.66
1:L:80:ASN:OD1	2:L:302:HOH:O	2.14	0.65
1:B:19:ILE:HD11	1:B:58:VAL:HG23	1.77	0.65
1:B:181:ALA:O	2:B:301:HOH:O	2.13	0.65
1:K:98:GLU:OE2	2:K:302:HOH:O	2.15	0.65
1:B:57:VAL:HB	1:B:84:VAL:HG22	1.79	0.65
1:P:179:ASN:ND2	2:P:306:HOH:O	2.30	0.64
1:L:187:LYS:HD3	1:L:188:ILE:H	1.62	0.64
1:N:143:ASP:OD2	1:N:170:VAL:N	2.24	0.64
1:D:60:THR:HG21	1:D:94:MET:HG2	1.79	0.64
1:C:162:GLN:NE2	1:E:165:ALA:O	2.29	0.64
1:K:46:MET:HE3	1:K:170:VAL:HA	1.78	0.63
1:B:162:GLN:NE2	1:F:165:ALA:O	2.28	0.63
1:H:171:GLU:OE2	1:H:197:LEU:HD21	1.98	0.63
1:I:185:GLU:OE1	2:I:305:HOH:O	2.15	0.63
1:B:85:LYS:HD3	1:B:102:HIS:CE1	2.33	0.63
1:F:112:SER:OG	2:F:303:HOH:O	2.16	0.63
1:D:29:PHE:CD1	1:D:118:ILE:HD11	2.33	0.63
1:J:8:LYS:N	2:J:307:HOH:O	2.31	0.63
1:L:171:GLU:OE2	1:L:197:LEU:HD21	1.98	0.62
1:P:14:LEU:HD23	1:P:16:GLN:H	1.64	0.62
1:M:8:LYS:N	2:M:305:HOH:O	2.33	0.62
1:N:87:PHE:CE2	1:N:98:GLU:HG2	2.29	0.62
1:L:102:HIS:CD2	1:L:107:MET:HE2	2.35	0.62
1:P:78:LEU:HD12	1:P:84:VAL:HG21	1.82	0.62
1:F:27:GLU:OE2	1:F:30:ARG:NH2	2.30	0.61
1:G:23:CYS:HA	1:G:60:THR:HG22	1.81	0.61
1:C:126:GLN:NE2	1:E:175:PHE:O	2.32	0.61
1:K:57:VAL:HB	1:K:84:VAL:HG22	1.82	0.60
1:C:29:PHE:CD2	1:C:118:ILE:HD11	2.36	0.60
1:L:23:CYS:HA	1:L:60:THR:HG22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:166:TYR:HA	1:O:162:GLN:HE22	1.67	0.60
1:C:73:GLU:OE2	1:C:73:GLU:N	2.22	0.60
1:N:63:TYR:HB3	1:N:67:LEU:HG	1.83	0.59
1:H:30:ARG:HA	1:H:36:LEU:HD22	1.85	0.59
1:D:165:ALA:O	1:J:162:GLN:NE2	2.30	0.59
1:P:57:VAL:HB	1:P:84:VAL:HG22	1.83	0.59
1:B:136:TYR:O	2:B:303:HOH:O	2.17	0.59
1:K:76:LYS:NZ	2:K:305:HOH:O	2.36	0.59
1:N:27:GLU:OE2	1:N:30:ARG:NE	2.31	0.59
1:O:59:VAL:HB	1:O:86:ILE:HG13	1.84	0.59
1:G:30:ARG:HA	1:G:36:LEU:HD22	1.84	0.59
1:I:63:TYR:HB3	1:I:67:LEU:HD13	1.84	0.59
1:E:75:SER:OG	2:E:302:HOH:O	2.16	0.58
1:C:57:VAL:HB	1:C:84:VAL:HG22	1.83	0.58
1:D:198:LYS:NZ	2:D:305:HOH:O	2.35	0.58
1:J:24:ASP:OD1	1:J:60:THR:HG23	2.03	0.58
1:O:63:TYR:HB3	1:O:67:LEU:HD12	1.86	0.58
1:J:12:HIS:O	2:J:305:HOH:O	2.17	0.58
1:P:100:GLU:OE1	2:P:305:HOH:O	2.17	0.58
1:C:107:MET:HB2	1:C:110:ARG:HG3	1.86	0.57
1:K:63:TYR:HE1	1:K:66:ARG:HB3	1.69	0.57
1:A:57:VAL:HB	1:A:84:VAL:HG22	1.86	0.57
1:M:123[A]:CYS:SG	1:M:124:VAL:N	2.78	0.57
1:K:205:THR:HG22	2:K:371:HOH:O	2.05	0.57
1:G:165:ALA:O	1:L:162:GLN:NE2	2.34	0.57
1:H:162:GLN:NE2	1:L:165:ALA:O	2.36	0.57
1:H:94:MET:HE3	1:H:127:THR:HG21	1.87	0.57
1:H:182:SER:HB3	1:M:90:MET:HG3	1.86	0.56
1:C:171:GLU:OE2	2:C:304:HOH:O	2.18	0.56
1:H:179:ASN:HD21	1:M:91:LYS:HE3	1.70	0.56
1:M:119:GLU:HG2	1:M:147:SER:HA	1.87	0.56
1:P:21:PHE:HD2	1:P:94:MET:HE3	1.70	0.56
1:E:24:ASP:OD1	1:E:60:THR:HG23	2.06	0.56
1:P:165:ALA:O	1:O:162:GLN:NE2	2.38	0.56
1:E:30:ARG:HA	1:E:36:LEU:HD22	1.88	0.56
1:L:23:CYS:HB2	1:L:94:MET:SD	2.45	0.55
1:D:63:TYR:HA	1:D:90:MET:HE1	1.87	0.55
1:J:119:GLU:HG2	1:J:147:SER:HA	1.89	0.55
1:B:21:PHE:HZ	1:B:103:LEU:HD11	1.70	0.55
1:D:9:ARG:NH2	2:D:306:HOH:O	2.39	0.55
1:I:24:ASP:OD1	1:I:60:THR:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:LYS:HD3	1:D:102:HIS:CE1	2.42	0.54
1:M:23:CYS:SG	1:M:123[B]:CYS:HB3	2.47	0.54
1:A:186:PHE:HE1	1:P:92:PHE:HZ	1.55	0.54
1:O:24:ASP:OD1	1:O:60:THR:HG23	2.07	0.54
1:B:182:SER:HB3	1:E:90:MET:HG3	1.89	0.54
1:F:51:LYS:NZ	1:F:80:ASN:HD22	2.04	0.54
1:E:51:LYS:HD3	1:E:81:VAL:HG22	1.90	0.54
1:G:171:GLU:OE2	1:G:197:LEU:HD21	2.07	0.54
1:H:94:MET:CE	1:H:127:THR:HG21	2.37	0.54
1:J:8:LYS:NZ	1:I:133:ASP:O	2.40	0.54
1:E:51:LYS:HG2	1:E:81:VAL:HG13	1.90	0.54
1:P:124:VAL:HG12	1:P:160:MET:HE1	1.89	0.54
1:H:60:THR:HG21	1:H:94:MET:HG2	1.90	0.54
1:C:19:ILE:HD13	1:C:107:MET:HE2	1.90	0.54
1:D:24:ASP:OD1	1:D:60:THR:HG23	2.08	0.54
1:D:171:GLU:OE2	1:D:197:LEU:HD21	2.08	0.54
1:C:28:VAL:HG11	1:C:67:LEU:HD22	1.88	0.54
1:D:195:GLU:OE2	1:D:198:LYS:NZ	2.39	0.53
1:J:60:THR:HG21	1:J:94:MET:HG2	1.90	0.53
1:N:190:SER:O	1:N:194:LYS:HG2	2.09	0.53
1:P:24:ASP:OD1	1:P:60:THR:HG23	2.09	0.53
1:P:87:PHE:CE2	1:P:98:GLU:HG2	2.44	0.53
1:J:8:LYS:HA	2:J:371:HOH:O	2.09	0.53
1:L:63:TYR:CZ	1:L:66:ARG:HG3	2.44	0.52
1:I:165:ALA:O	1:K:162:GLN:NE2	2.38	0.52
1:E:57:VAL:HB	1:E:84:VAL:HG22	1.91	0.52
1:P:156:ALA:O	1:P:160:MET:HG3	2.09	0.52
1:C:60:THR:HG21	1:C:94:MET:HG2	1.92	0.52
1:M:85:LYS:HB3	1:M:87:PHE:CE1	2.44	0.52
1:F:15:PRO:HG2	1:F:16:GLN:HE22	1.74	0.52
1:L:30:ARG:HB3	1:N:37:PRO:HG2	1.91	0.52
1:N:12:HIS:O	2:N:304:HOH:O	2.19	0.52
1:F:59:VAL:HB	1:F:86:ILE:HG12	1.90	0.52
1:A:63:TYR:CE1	1:A:90:MET:HE1	2.45	0.51
1:C:9:ARG:NH1	2:C:306:HOH:O	2.38	0.51
1:G:63:TYR:HB3	1:G:67:LEU:HD13	1.92	0.51
1:K:24:ASP:OD1	1:K:60:THR:HG23	2.10	0.51
1:G:19:ILE:HD11	1:G:58:VAL:HG23	1.90	0.51
1:L:107:MET:HB2	1:L:110:ARG:HG3	1.91	0.51
1:P:21:PHE:CD2	1:P:94:MET:HE3	2.45	0.51
1:C:24:ASP:OD1	1:C:60:THR:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:GLN:NE2	1:N:165:ALA:O	2.40	0.51
1:M:30:ARG:HA	1:M:36:LEU:HD22	1.92	0.51
1:P:94:MET:HE2	1:P:127:THR:HG21	1.93	0.51
1:O:118:ILE:HG22	1:O:146:SER:O	2.11	0.51
1:E:65:SER:N	2:E:303:HOH:O	2.35	0.51
1:G:23:CYS:HB2	1:G:94:MET:SD	2.50	0.51
1:G:73:GLU:OE1	1:G:73:GLU:N	2.33	0.51
1:H:98:GLU:CD	1:H:98:GLU:H	2.18	0.51
1:D:114:LEU:HD23	1:D:139:HIS:HB2	1.92	0.51
1:D:183:ASN:HB3	1:D:185:GLU:OE2	2.10	0.51
1:O:24:ASP:HA	1:O:26:GLN:HE22	1.76	0.51
1:L:80:ASN:HB3	1:B:109:GLN:HG3	1.92	0.50
1:C:165:ALA:O	1:F:162:GLN:NE2	2.38	0.50
1:E:171:GLU:OE2	1:E:197:LEU:HD21	2.10	0.50
1:N:104:THR:O	1:N:108:PRO:HG3	2.11	0.50
1:I:195:GLU:HA	1:I:198:LYS:HD2	1.93	0.50
1:O:23:CYS:HA	1:O:60:THR:HG22	1.93	0.50
1:F:195:GLU:HA	1:F:198:LYS:HD2	1.93	0.50
1:H:143:ASP:OD1	2:H:301:HOH:O	2.19	0.50
1:D:40:ILE:HD13	1:D:71:VAL:HG21	1.94	0.50
1:G:114:LEU:HD11	1:G:177:LEU:HD11	1.94	0.50
1:H:19:ILE:HD11	1:H:58:VAL:HG23	1.92	0.50
1:F:51:LYS:HZ3	1:F:80:ASN:HD22	1.58	0.50
1:O:140:VAL:HG21	1:O:160:MET:HE2	1.93	0.50
1:G:91:LYS:HG2	1:M:180:ASP:OD2	2.12	0.50
1:L:24:ASP:OD1	1:L:60:THR:HG23	2.12	0.50
1:A:162:GLN:HE22	1:N:166:TYR:HA	1.77	0.50
1:B:90:MET:HE3	1:F:181:ALA:HB3	1.93	0.49
1:L:79:GLU:O	1:B:16:GLN:HG3	2.11	0.49
1:J:166:TYR:HA	1:I:162:GLN:HE22	1.77	0.49
1:B:19:ILE:HD12	1:B:56:PRO:HB2	1.93	0.49
1:F:28:VAL:HG11	1:F:67:LEU:HD22	1.93	0.49
1:E:16:GLN:CD	1:E:16:GLN:H	2.19	0.49
1:M:63:TYR:CE2	1:M:90:MET:HE1	2.48	0.49
1:M:113:VAL:HG21	1:M:131:LEU:HD13	1.93	0.49
1:B:176:GLN:HG2	2:B:365:HOH:O	2.11	0.49
1:D:29:PHE:HA	1:D:32:LEU:HD12	1.95	0.49
1:N:51:LYS:NZ	1:N:80:ASN:HB2	2.28	0.49
1:N:185:GLU:H	1:N:185:GLU:CD	2.14	0.49
1:P:89:LYS:HE2	1:P:91:LYS:O	2.12	0.49
1:D:23:CYS:HA	1:D:60:THR:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:171:GLU:CD	1:P:197:LEU:HD21	2.37	0.49
1:H:52:LEU:HD22	1:H:188:ILE:HG12	1.95	0.48
1:A:100:GLU:OE2	1:A:134:LYS:HE3	2.13	0.48
1:O:28:VAL:HG21	1:O:67:LEU:HD23	1.94	0.48
1:I:81:VAL:HB	1:I:84:VAL:CG2	2.42	0.48
1:C:118:ILE:HG22	1:C:146:SER:H	1.79	0.48
1:E:175:PHE:HE1	1:E:186:PHE:HE1	1.61	0.48
1:H:162:GLN:HE22	1:L:166:TYR:HA	1.79	0.48
1:M:19:ILE:HD12	1:M:107:MET:SD	2.53	0.48
1:C:33:THR:HB	1:C:36:LEU:HB2	1.95	0.48
1:D:166:TYR:HA	1:J:162:GLN:HE22	1.79	0.48
1:A:165:ALA:O	1:P:162:GLN:NE2	2.43	0.48
1:G:133:ASP:OD1	1:M:8:LYS:HE3	2.12	0.48
1:N:123[A]:CYS:SG	2:N:364:HOH:O	2.61	0.48
1:G:76:LYS:O	1:G:79:GLU:HG3	2.13	0.48
1:N:72:SER:OG	2:N:303:HOH:O	2.13	0.48
1:L:106:ASN:OD1	1:E:134:LYS:HE2	2.14	0.48
1:P:143:ASP:OD1	1:P:143:ASP:N	2.44	0.48
1:N:107:MET:HE2	1:N:107:MET:HB3	1.80	0.48
1:G:52:LEU:HD21	1:G:188:ILE:HG12	1.95	0.47
1:D:162:GLN:HE22	1:K:166:TYR:HA	1.79	0.47
1:A:23:CYS:HA	1:A:60:THR:HG22	1.96	0.47
1:P:19:ILE:HD11	1:P:58:VAL:HG23	1.96	0.47
1:O:24:ASP:HA	1:O:26:GLN:NE2	2.29	0.47
1:D:79:GLU:OE1	2:D:302:HOH:O	2.20	0.47
1:J:118:ILE:HG22	1:J:146:SER:O	2.15	0.47
1:O:193:ILE:O	1:O:197:LEU:HD12	2.13	0.47
1:N:59:VAL:HB	1:N:86:ILE:HG12	1.96	0.47
1:K:85:LYS:HG3	1:K:102:HIS:CE1	2.49	0.47
1:N:187:LYS:NZ	2:N:310:HOH:O	2.47	0.47
1:C:51:LYS:HG3	1:C:81:VAL:HG22	1.97	0.47
1:E:143:ASP:HB2	1:E:170:VAL:HG23	1.96	0.47
1:P:123[B]:CYS:HB2	2:P:353:HOH:O	2.15	0.47
1:N:85:LYS:HG2	1:N:87:PHE:CE1	2.50	0.47
1:M:146:SER:HA	1:M:153:ARG:HD2	1.96	0.47
1:J:15:PRO:O	1:J:110:ARG:NH1	2.48	0.47
1:J:120:THR:HG23	1:J:145:VAL:HB	1.97	0.47
1:I:60:THR:HG21	1:I:94:MET:HG2	1.96	0.47
1:P:8:LYS:HE2	1:O:133:ASP:HA	1.96	0.47
1:P:155:MET:HE3	1:P:155:MET:HB3	1.82	0.47
1:H:75:SER:HA	1:H:78:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ILE:HD11	1:A:58:VAL:HG23	1.95	0.47
1:P:175:PHE:CZ	1:P:193:ILE:HD13	2.50	0.47
1:O:107:MET:HE2	1:O:110:ARG:HD2	1.97	0.47
1:G:24:ASP:OD1	1:G:60:THR:HG23	2.15	0.46
1:P:46:MET:HE2	1:P:114:LEU:HD12	1.97	0.46
1:P:33:THR:HB	1:P:36:LEU:HB2	1.97	0.46
1:O:56:PRO:HG2	1:O:107:MET:HE1	1.97	0.46
1:N:72:SER:O	1:N:76:LYS:HG3	2.15	0.46
1:K:41:HIS:CD2	1:K:199:VAL:HG21	2.51	0.46
1:B:171:GLU:OE2	1:B:197:LEU:HD11	2.15	0.46
1:I:125:LEU:HD11	1:I:159:ARG:HG2	1.98	0.46
1:K:123:CYS:SG	2:K:367:HOH:O	2.61	0.46
1:O:28:VAL:HG11	1:O:67:LEU:HD22	1.97	0.46
1:A:166:TYR:HA	1:P:162:GLN:HE22	1.80	0.46
1:O:14:LEU:HD23	1:O:16:GLN:NE2	2.31	0.46
1:E:55:LEU:HD11	1:E:177:LEU:HD13	1.98	0.46
1:E:97:PRO:HD2	1:E:98:GLU:OE2	2.15	0.46
1:G:143:ASP:HB2	1:G:170:VAL:HG23	1.96	0.46
1:P:94:MET:CE	1:P:127:THR:HG21	2.45	0.46
1:B:91:LYS:HA	1:F:180:ASP:HA	1.98	0.46
1:I:51:LYS:HE2	1:I:80:ASN:HB2	1.98	0.46
1:O:26:GLN:HE22	1:O:61:THR:HA	1.81	0.46
1:J:123:CYS:SG	2:J:377:HOH:O	2.51	0.45
1:P:115:LEU:HG	1:P:124:VAL:HG13	1.98	0.45
1:O:60:THR:HG21	1:O:94:MET:HG2	1.98	0.45
1:H:42:SER:HB3	1:H:170:VAL:HG21	1.99	0.45
1:C:193:ILE:HD13	1:C:193:ILE:HA	1.80	0.45
1:G:185:GLU:O	1:G:189:ILE:HG12	2.15	0.45
1:K:30:ARG:HA	1:K:36:LEU:HD23	1.99	0.45
1:F:24:ASP:OD1	1:F:60:THR:HG23	2.17	0.45
1:J:26:GLN:NE2	1:J:62:GLN:O	2.45	0.45
1:I:51:LYS:HE3	1:I:81:VAL:HG22	1.99	0.45
1:E:114:LEU:HD11	1:E:177:LEU:HD11	1.99	0.45
1:P:24:ASP:OD2	1:P:123[B]:CYS:SG	2.75	0.45
1:N:60:THR:HG22	1:N:87:PHE:HB2	1.98	0.45
1:K:60:THR:HG21	1:K:94:MET:CG	2.46	0.45
1:E:14:LEU:HB3	1:E:16:GLN:OE1	2.17	0.45
1:I:23:CYS:HA	1:I:60:THR:HG22	1.99	0.45
1:B:90:MET:HE3	1:B:90:MET:HB3	1.78	0.45
1:E:63:TYR:HA	1:E:90:MET:HE1	1.99	0.45
1:B:162:GLN:HG3	2:B:370:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:PHE:CE1	1:P:92:PHE:HZ	2.35	0.44
1:G:24:ASP:HA	1:G:26:GLN:HE22	1.82	0.44
1:J:63:TYR:HB3	2:J:316:HOH:O	2.16	0.44
1:P:23:CYS:SG	1:P:123[A]:CYS:HB3	2.58	0.44
1:B:185:GLU:O	1:B:189:ILE:HG13	2.16	0.44
1:E:23:CYS:HA	1:E:60:THR:HG22	1.99	0.44
1:G:195:GLU:OE2	1:G:198:LYS:HD2	2.18	0.44
1:B:161:ARG:HH11	1:E:162:GLN:HE21	1.65	0.44
1:C:46:MET:HE1	1:C:174:ILE:HG13	2.00	0.44
1:N:9:ARG:HG3	2:N:365:HOH:O	2.17	0.44
1:P:114:LEU:HD11	1:P:173:ALA:HB1	2.00	0.44
1:O:81:VAL:HB	1:O:84:VAL:CG2	2.48	0.44
1:I:114:LEU:HD23	1:I:139:HIS:HB2	2.00	0.44
1:A:114:LEU:HD23	1:A:139:HIS:HB2	2.00	0.44
1:J:53:LEU:HD21	1:J:189:ILE:HD11	2.00	0.44
1:P:87:PHE:CD2	1:P:98:GLU:HG2	2.52	0.44
1:G:121:HIS:HD1	1:G:121:HIS:H	1.65	0.43
1:O:85:LYS:HB3	1:O:87:PHE:CE1	2.53	0.43
1:M:184:PRO:O	2:M:302:HOH:O	2.21	0.43
1:P:95:LEU:HD12	1:P:95:LEU:HA	1.89	0.43
1:F:67:LEU:HD23	1:F:67:LEU:HA	1.89	0.43
1:G:81:VAL:HB	1:G:84:VAL:CG2	2.49	0.43
1:A:134:LYS:HD2	1:A:134:LYS:HA	1.77	0.43
1:O:85:LYS:HB3	1:O:87:PHE:CZ	2.53	0.43
1:C:13:LEU:HB2	1:C:176:GLN:HB3	1.99	0.43
1:A:111:LYS:HB2	2:A:364:HOH:O	2.18	0.43
1:E:95:LEU:HD12	1:E:95:LEU:HA	1.87	0.43
1:O:9:ARG:HG3	1:O:9:ARG:HH11	1.83	0.43
1:F:23:CYS:HA	1:F:60:THR:HG22	1.99	0.43
1:O:26:GLN:NE2	1:O:61:THR:HA	2.33	0.43
1:F:153:ARG:HD3	2:F:341:HOH:O	2.18	0.43
1:J:60:THR:HG21	1:J:94:MET:CG	2.48	0.43
1:O:186:PHE:HD1	1:O:187:LYS:HD2	1.84	0.43
1:A:52:LEU:HD13	1:A:188:ILE:HG23	2.01	0.43
1:G:161:ARG:HB2	1:G:167:ILE:CD1	2.49	0.43
1:M:123[B]:CYS:SG	2:M:365:HOH:O	2.62	0.43
1:D:29:PHE:CG	1:D:118:ILE:HD11	2.54	0.43
1:A:51:LYS:HD2	1:A:80:ASN:OD1	2.18	0.43
1:A:156:ALA:O	1:A:160:MET:HG3	2.19	0.43
1:F:28:VAL:HG13	1:F:29:PHE:CD1	2.53	0.43
1:M:27:GLU:O	1:M:30:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ILE:HD12	1:A:107:MET:SD	2.59	0.42
1:P:47:VAL:HG23	1:P:77:ASN:HD22	1.84	0.42
1:O:107:MET:CE	1:O:110:ARG:HD2	2.48	0.42
1:C:91:LYS:NZ	2:C:309:HOH:O	2.51	0.42
1:C:166:TYR:HA	1:F:162:GLN:NE2	2.34	0.42
1:J:59:VAL:HB	1:J:86:ILE:HG12	2.02	0.42
1:I:166:TYR:HA	1:K:162:GLN:HE22	1.85	0.42
1:P:59:VAL:O	1:P:86:ILE:HA	2.19	0.42
1:B:162:GLN:NE2	1:F:166:TYR:HA	2.35	0.42
1:L:134:LYS:HB3	1:L:134:LYS:HE3	1.76	0.42
1:K:199:VAL:HA	1:E:28:VAL:HA	2.01	0.42
1:K:23:CYS:SG	1:K:123:CYS:HB3	2.60	0.42
1:P:85:LYS:HE3	1:P:85:LYS:HB3	1.83	0.42
1:J:19:ILE:HD11	1:J:58:VAL:HG23	2.01	0.42
1:P:51:LYS:HE3	1:P:81:VAL:HG22	2.01	0.42
1:P:125:LEU:HD23	1:P:160:MET:HG2	2.02	0.42
1:D:162:GLN:NE2	1:K:166:TYR:HA	2.34	0.42
1:L:63:TYR:HB3	1:L:67:LEU:HD23	2.02	0.42
1:D:190:SER:O	1:D:194:LYS:HD3	2.20	0.42
1:A:19:ILE:HG23	1:A:113:VAL:HG22	2.01	0.42
1:C:76:LYS:O	1:C:79:GLU:HG3	2.19	0.42
1:C:84:VAL:C	1:C:85:LYS:HD2	2.45	0.42
1:H:107:MET:HE2	1:H:107:MET:HB3	1.85	0.42
1:I:60:THR:HG22	1:I:94:MET:HE3	2.02	0.42
1:I:168:THR:OG1	1:I:169:SER:N	2.53	0.42
1:A:60:THR:HG21	1:A:94:MET:HG2	2.02	0.42
1:B:201:ASN:HB3	1:B:204:ASP:HB2	2.02	0.42
1:A:33:THR:HB	1:A:36:LEU:HB2	2.02	0.42
1:O:51:LYS:HG3	1:O:81:VAL:HG22	2.01	0.41
1:O:182:SER:OG	1:N:90:MET:HG2	2.20	0.41
1:B:123:CYS:SG	2:B:374:HOH:O	2.62	0.41
1:C:102:HIS:O	1:C:106:ASN:HB2	2.20	0.41
1:A:76:LYS:HA	1:A:79:GLU:OE2	2.20	0.41
1:G:107:MET:HE2	1:G:107:MET:HB3	1.97	0.41
1:J:166:TYR:HA	1:I:162:GLN:NE2	2.36	0.41
1:K:26:GLN:HB3	1:K:67:LEU:O	2.19	0.41
1:C:117:GLY:O	1:C:145:VAL:HA	2.21	0.41
1:E:63:TYR:CD1	1:E:90:MET:HE1	2.55	0.41
1:C:115:LEU:HG	1:C:124:VAL:HG13	2.02	0.41
1:L:85:LYS:HD3	1:L:85:LYS:HA	1.64	0.41
1:L:95:LEU:HD12	1:L:95:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:102:HIS:CD2	1:L:102:HIS:C	2.99	0.41
1:D:9:ARG:HA	1:D:9:ARG:NE	2.35	0.41
1:I:19:ILE:HD11	1:I:58:VAL:HG23	2.01	0.41
1:O:9:ARG:HG3	1:O:9:ARG:NH1	2.35	0.41
1:B:95:LEU:HD12	1:B:95:LEU:HA	1.97	0.41
1:C:53:LEU:HD21	1:C:189:ILE:HD11	2.02	0.41
1:C:63:TYR:HB3	1:C:67:LEU:HD12	2.02	0.41
1:P:85:LYS:HB2	1:P:87:PHE:CE1	2.55	0.41
1:F:90:MET:HE3	1:F:90:MET:HB3	1.96	0.41
1:P:199:VAL:HA	2:P:312:HOH:O	2.19	0.41
1:H:146:SER:HA	1:H:153:ARG:HD2	2.02	0.41
1:L:100:GLU:OE1	1:L:134:LYS:HE2	2.21	0.41
1:M:76:LYS:O	1:M:79:GLU:HB2	2.21	0.41
1:M:102:HIS:O	1:M:106:ASN:HB2	2.20	0.41
1:J:95:LEU:HA	1:J:95:LEU:HD12	1.80	0.41
1:K:46:MET:HE1	1:K:174:ILE:HG13	2.03	0.41
1:P:44:ASN:OD1	1:P:74:ILE:HA	2.20	0.41
1:G:119:GLU:OE2	1:G:148:SER:N	2.51	0.41
1:J:120:THR:HA	1:J:124:VAL:HB	2.03	0.41
1:P:166:TYR:HA	1:O:162:GLN:NE2	2.34	0.41
1:P:187:LYS:HA	1:P:187:LYS:HD2	1.96	0.41
1:E:30:ARG:HA	1:E:36:LEU:CD2	2.50	0.41
1:E:155:MET:HE3	1:E:155:MET:HB3	1.98	0.41
1:A:143:ASP:OD1	1:A:143:ASP:N	2.52	0.41
1:B:143:ASP:HB2	1:B:170:VAL:HG23	2.01	0.41
1:F:19:ILE:HD11	1:F:58:VAL:HG23	2.02	0.41
1:I:33:THR:HG21	1:I:118:ILE:HG21	2.03	0.40
1:P:179:ASN:HD22	1:P:179:ASN:C	2.29	0.40
1:B:119:GLU:OE2	1:B:148:SER:N	2.54	0.40
1:L:63:TYR:HE1	1:L:65:SER:HG	1.69	0.40
1:D:22:VAL:HB	1:D:59:VAL:HG22	2.03	0.40
1:A:102:HIS:O	1:A:106:ASN:HB2	2.21	0.40
1:A:165:ALA:C	1:P:162:GLN:HE22	2.28	0.40
1:A:181:ALA:HA	1:A:186:PHE:CG	2.56	0.40
1:P:107:MET:HE2	1:P:107:MET:HB3	1.83	0.40
1:E:13:LEU:HB2	1:E:176:GLN:HB3	2.04	0.40
1:G:76:LYS:HE3	1:G:76:LYS:HB3	1.87	0.40
1:H:98:GLU:CD	1:H:98:GLU:N	2.79	0.40
1:K:162:GLN:HG3	2:K:370:HOH:O	2.20	0.40
1:O:191:LYS:O	1:O:195:GLU:HG2	2.21	0.40
1:N:61:THR:OG1	1:N:88:ASP:OD2	2.27	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ARG:NH1	1:E:162:GLN:HE21	2.18	0.40
1:G:166:TYR:HA	1:L:162:GLN:HE22	1.85	0.40
1:H:149:THR:HB	1:L:204:ASP:OD2	2.21	0.40
1:I:143:ASP:OD1	1:I:143:ASP:N	2.46	0.40
1:K:63:TYR:CE1	1:K:65:SER:HB3	2.57	0.40
1:A:95:LEU:HD12	1:A:95:LEU:HA	1.95	0.40
1:P:103:LEU:HD12	1:P:136:TYR:HE2	1.86	0.40
1:G:166:TYR:HA	1:L:162:GLN:NE2	2.36	0.40
1:H:114:LEU:HD13	1:H:139:HIS:HB2	2.03	0.40
1:L:187:LYS:HD3	1:L:188:ILE:N	2.31	0.40
1:B:162:GLN:HE22	1:F:166:TYR:HA	1.87	0.40
1:F:23:CYS:SG	1:F:123:CYS:HB3	2.62	0.40
1:F:125:LEU:HD11	1:F:159:ARG:HG2	2.02	0.40
1:F:143:ASP:HB2	1:F:170:VAL:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	199/209 (95%)	191 (96%)	8 (4%)	0	100	100
1	B	196/209 (94%)	194 (99%)	2 (1%)	0	100	100
1	C	196/209 (94%)	190 (97%)	6 (3%)	0	100	100
1	D	196/209 (94%)	191 (97%)	5 (3%)	0	100	100
1	E	196/209 (94%)	193 (98%)	3 (2%)	0	100	100
1	F	196/209 (94%)	194 (99%)	2 (1%)	0	100	100
1	G	196/209 (94%)	192 (98%)	4 (2%)	0	100	100
1	H	196/209 (94%)	191 (97%)	5 (3%)	0	100	100
1	I	196/209 (94%)	191 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	196/209 (94%)	190 (97%)	6 (3%)	0	100	100
1	K	192/209 (92%)	183 (95%)	9 (5%)	0	100	100
1	L	197/209 (94%)	190 (96%)	7 (4%)	0	100	100
1	M	197/209 (94%)	192 (98%)	5 (2%)	0	100	100
1	N	197/209 (94%)	191 (97%)	6 (3%)	0	100	100
1	O	197/209 (94%)	193 (98%)	4 (2%)	0	100	100
1	P	197/209 (94%)	196 (100%)	1 (0%)	0	100	100
All	All	3140/3344 (94%)	3062 (98%)	78 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	181/188 (96%)	178 (98%)	3 (2%)	53	72
1	B	181/188 (96%)	178 (98%)	3 (2%)	53	72
1	C	181/188 (96%)	176 (97%)	5 (3%)	38	56
1	D	181/188 (96%)	178 (98%)	3 (2%)	53	72
1	E	181/188 (96%)	176 (97%)	5 (3%)	38	56
1	F	181/188 (96%)	177 (98%)	4 (2%)	45	65
1	G	180/188 (96%)	175 (97%)	5 (3%)	38	56
1	H	181/188 (96%)	180 (99%)	1 (1%)	78	89
1	I	181/188 (96%)	178 (98%)	3 (2%)	53	72
1	J	181/188 (96%)	177 (98%)	4 (2%)	45	65
1	K	179/188 (95%)	174 (97%)	5 (3%)	38	56
1	L	182/188 (97%)	177 (97%)	5 (3%)	39	58
1	M	182/188 (97%)	178 (98%)	4 (2%)	45	65
1	N	182/188 (97%)	176 (97%)	6 (3%)	33	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	O	182/188 (97%)	179 (98%)	3 (2%)	55 73
1	P	179/188 (95%)	171 (96%)	8 (4%)	24 37
All	All	2895/3008 (96%)	2828 (98%)	67 (2%)	45 63

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	23	CYS
1	G	111	LYS
1	G	120	THR
1	G	123	CYS
1	G	148	SER
1	H	120	THR
1	L	23	CYS
1	L	120	THR
1	L	123[A]	CYS
1	L	123[B]	CYS
1	L	199	VAL
1	M	85	LYS
1	M	120	THR
1	M	123[A]	CYS
1	M	123[B]	CYS
1	D	57	VAL
1	D	120	THR
1	D	180	ASP
1	J	28	VAL
1	J	91	LYS
1	J	105	SER
1	J	120	THR
1	I	84	VAL
1	I	120	THR
1	I	199	VAL
1	K	14	LEU
1	K	120	THR
1	K	131	LEU
1	K	162	GLN
1	K	199	VAL
1	A	120	THR
1	A	190	SER
1	A	199	VAL
1	P	65	SER

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Mol	Chain	Res	Type
1	P	75	SER
1	P	110	ARG
1	P	120	THR
1	P	125	LEU
1	P	148	SER
1	P	190	SER
1	P	193	ILE
1	O	120	THR
1	O	123[A]	CYS
1	O	123[B]	CYS
1	N	23	CYS
1	N	84	VAL
1	N	90	MET
1	N	120	THR
1	N	143	ASP
1	N	162	GLN
1	B	120	THR
1	B	162	GLN
1	B	197	LEU
1	C	118	ILE
1	C	120	THR
1	C	125	LEU
1	C	189	ILE
1	C	197	LEU
1	F	17	SER
1	F	75	SER
1	F	120	THR
1	F	190	SER
1	E	17	SER
1	E	53	LEU
1	E	67	LEU
1	E	120	THR
1	E	191	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	26	GLN
1	G	41	HIS
1	G	101	HIS
1	G	106	ASN
1	H	12	HIS

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Mol	Chain	Res	Type
1	H	179	ASN
1	L	12	HIS
1	L	54	ASN
1	L	102	HIS
1	M	102	HIS
1	M	106	ASN
1	M	176	GLN
1	D	12	HIS
1	D	80	ASN
1	J	179	ASN
1	I	101	HIS
1	K	12	HIS
1	K	41	HIS
1	K	77	ASN
1	K	102	HIS
1	K	106	ASN
1	K	179	ASN
1	A	16	GLN
1	P	101	HIS
1	P	139	HIS
1	P	162	GLN
1	P	179	ASN
1	O	26	GLN
1	O	41	HIS
1	O	80	ASN
1	O	82	ASN
1	O	162	GLN
1	N	12	HIS
1	N	101	HIS
1	N	106	ASN
1	B	12	HIS
1	C	35	GLN
1	C	101	HIS
1	C	102	HIS
1	C	183	ASN
1	F	12	HIS
1	F	16	GLN
1	F	80	ASN
1	F	102	HIS
1	F	106	ASN
1	E	41	HIS
1	E	162	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	201/209 (96%)	-0.17	2 (0%) 79 80	25, 33, 53, 69	0
1	B	198/209 (94%)	-0.04	2 (1%) 79 80	27, 38, 54, 71	0
1	C	198/209 (94%)	0.16	1 (0%) 87 87	32, 45, 69, 90	0
1	D	198/209 (94%)	-0.11	4 (2%) 65 66	25, 36, 60, 74	0
1	E	198/209 (94%)	0.09	1 (0%) 87 87	30, 44, 65, 73	0
1	F	198/209 (94%)	0.17	5 (2%) 58 60	31, 46, 68, 96	0
1	G	198/209 (94%)	0.12	6 (3%) 52 54	27, 42, 74, 87	0
1	H	198/209 (94%)	0.08	2 (1%) 79 80	28, 44, 63, 77	0
1	I	198/209 (94%)	-0.24	0 100 100	24, 34, 54, 73	0
1	J	198/209 (94%)	-0.20	0 100 100	24, 36, 57, 65	0
1	K	196/209 (93%)	-0.08	5 (2%) 57 59	21, 36, 59, 77	0
1	L	198/209 (94%)	0.03	2 (1%) 79 80	20, 40, 66, 86	1 (0%)
1	M	198/209 (94%)	0.05	4 (2%) 65 66	21, 40, 59, 69	1 (0%)
1	N	198/209 (94%)	0.12	2 (1%) 79 80	23, 45, 69, 91	1 (0%)
1	O	198/209 (94%)	0.20	4 (2%) 65 66	22, 47, 71, 84	1 (0%)
1	P	198/209 (94%)	0.36	5 (2%) 58 60	22, 53, 77, 96	1 (0%)
All	All	3169/3344 (94%)	0.03	45 (1%) 73 75	20, 41, 66, 96	5 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	29	PHE	4.5
1	E	205	THR	3.7
1	K	205	THR	3.3
1	P	205	THR	3.0
1	H	205	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	O	178	ALA	2.9
1	G	28	VAL	2.9
1	P	14	LEU	2.7
1	G	67	LEU	2.7
1	O	118	ILE	2.7
1	C	205	THR	2.7
1	H	65	SER	2.7
1	F	66	ARG	2.7
1	D	9	ARG	2.5
1	P	180	ASP	2.5
1	M	123[A]	CYS	2.5
1	P	82	ASN	2.4
1	D	181	ALA	2.4
1	A	63	TYR	2.4
1	K	83	ASP	2.4
1	A	29	PHE	2.3
1	P	178	ALA	2.3
1	M	65	SER	2.3
1	F	205	THR	2.3
1	G	63	TYR	2.2
1	K	186	PHE	2.2
1	M	188	ILE	2.2
1	G	80	ASN	2.2
1	D	180	ASP	2.2
1	B	80	ASN	2.2
1	L	205	THR	2.2
1	D	205	THR	2.2
1	N	205	THR	2.2
1	F	178	ALA	2.2
1	O	112	SER	2.1
1	M	205	THR	2.1
1	K	65	SER	2.1
1	O	67	LEU	2.1
1	G	68	GLY	2.1
1	N	143	ASP	2.0
1	B	143	ASP	2.0
1	K	28	VAL	2.0
1	L	80	ASN	2.0
1	F	143	ASP	2.0
1	F	179	ASN	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 oligosaccharides 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.