



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:44 AM UTC

PDB ID : 4YNN / pdb_00004ynn
Title : Structure of Legionella pneumophila DegQ (S190A variant)
Authors : Wrase, R.; Hilgenfeld, R.; Hansen, G.
Deposited on : 2015-03-10
Resolution : 3.20 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

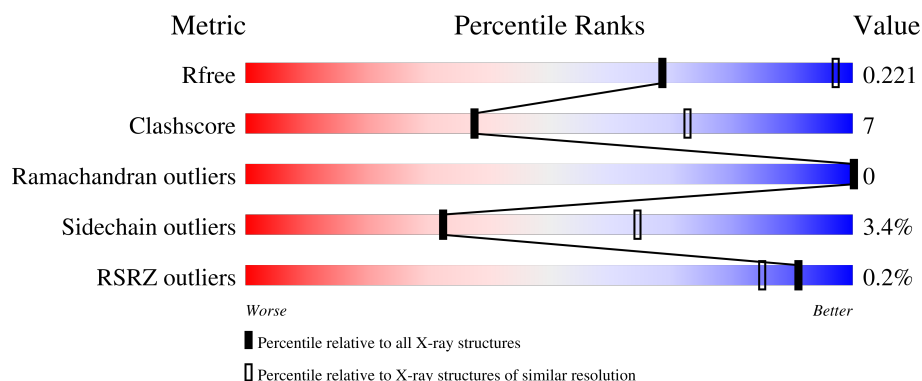
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.



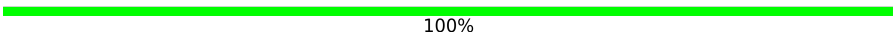
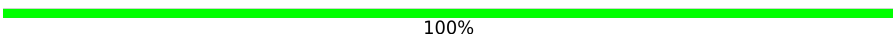
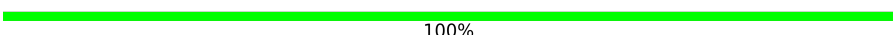
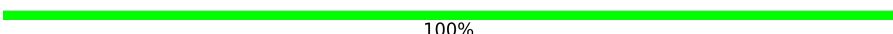
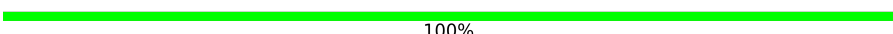
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	448	 70% 18% • 11%
1	B	448	 73% 16% 11%
1	C	448	 72% 17% • 11%
1	D	448	 71% 18% • 11%
1	E	448	 71% 17% • 11%

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Mol	Chain	Length	Quality of chain
1	F	448	
1	G	448	
1	H	448	
2	I	8	
3	J	6	
3	L	6	
4	K	7	
4	M	7	
4	N	7	
4	O	7	
4	P	7	
5	Q	3	
5	R	3	
5	S	3	
5	T	3	
5	U	3	
5	V	3	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24195 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 Protease DO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			2979	1885	523	566	5			
1	B	399	Total	C	N	O	S	0	0	0
			2971	1880	522	565	4			
1	C	400	Total	C	N	O	S	0	0	0
			2979	1885	523	566	5			
1	D	400	Total	C	N	O	S	0	0	0
			2979	1885	523	566	5			
1	E	400	Total	C	N	O	S	0	0	0
			2979	1885	523	566	5			
1	F	400	Total	C	N	O	S	0	0	0
			2979	1885	523	566	5			
1	G	400	Total	C	N	O	S	0	0	0
			2979	1885	523	566	5			
1	H	400	Total	C	N	O	S	0	0	0
			2979	1885	523	566	5			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP Q5ZVV9
A	-10	ARG	-	expression tag	UNP Q5ZVV9
A	-9	GLY	-	expression tag	UNP Q5ZVV9
A	-8	SER	-	expression tag	UNP Q5ZVV9
A	-7	HIS	-	expression tag	UNP Q5ZVV9
A	-6	HIS	-	expression tag	UNP Q5ZVV9
A	-5	HIS	-	expression tag	UNP Q5ZVV9
A	-4	HIS	-	expression tag	UNP Q5ZVV9
A	-3	HIS	-	expression tag	UNP Q5ZVV9
A	-2	HIS	-	expression tag	UNP Q5ZVV9
A	-1	GLY	-	expression tag	UNP Q5ZVV9
A	0	SER	-	expression tag	UNP Q5ZVV9
A	190	ALA	SER	engineered mutation	UNP Q5ZVV9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	MET	-	initiating methionine	UNP Q5ZVV9
B	-10	ARG	-	expression tag	UNP Q5ZVV9
B	-9	GLY	-	expression tag	UNP Q5ZVV9
B	-8	SER	-	expression tag	UNP Q5ZVV9
B	-7	HIS	-	expression tag	UNP Q5ZVV9
B	-6	HIS	-	expression tag	UNP Q5ZVV9
B	-5	HIS	-	expression tag	UNP Q5ZVV9
B	-4	HIS	-	expression tag	UNP Q5ZVV9
B	-3	HIS	-	expression tag	UNP Q5ZVV9
B	-2	HIS	-	expression tag	UNP Q5ZVV9
B	-1	GLY	-	expression tag	UNP Q5ZVV9
B	0	SER	-	expression tag	UNP Q5ZVV9
B	190	ALA	SER	engineered mutation	UNP Q5ZVV9
C	-11	MET	-	initiating methionine	UNP Q5ZVV9
C	-10	ARG	-	expression tag	UNP Q5ZVV9
C	-9	GLY	-	expression tag	UNP Q5ZVV9
C	-8	SER	-	expression tag	UNP Q5ZVV9
C	-7	HIS	-	expression tag	UNP Q5ZVV9
C	-6	HIS	-	expression tag	UNP Q5ZVV9
C	-5	HIS	-	expression tag	UNP Q5ZVV9
C	-4	HIS	-	expression tag	UNP Q5ZVV9
C	-3	HIS	-	expression tag	UNP Q5ZVV9
C	-2	HIS	-	expression tag	UNP Q5ZVV9
C	-1	GLY	-	expression tag	UNP Q5ZVV9
C	0	SER	-	expression tag	UNP Q5ZVV9
C	190	ALA	SER	engineered mutation	UNP Q5ZVV9
D	-11	MET	-	initiating methionine	UNP Q5ZVV9
D	-10	ARG	-	expression tag	UNP Q5ZVV9
D	-9	GLY	-	expression tag	UNP Q5ZVV9
D	-8	SER	-	expression tag	UNP Q5ZVV9
D	-7	HIS	-	expression tag	UNP Q5ZVV9
D	-6	HIS	-	expression tag	UNP Q5ZVV9
D	-5	HIS	-	expression tag	UNP Q5ZVV9
D	-4	HIS	-	expression tag	UNP Q5ZVV9
D	-3	HIS	-	expression tag	UNP Q5ZVV9
D	-2	HIS	-	expression tag	UNP Q5ZVV9
D	-1	GLY	-	expression tag	UNP Q5ZVV9
D	0	SER	-	expression tag	UNP Q5ZVV9
D	190	ALA	SER	engineered mutation	UNP Q5ZVV9
E	-11	MET	-	initiating methionine	UNP Q5ZVV9
E	-10	ARG	-	expression tag	UNP Q5ZVV9
E	-9	GLY	-	expression tag	UNP Q5ZVV9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-8	SER	-	expression tag	UNP Q5ZVV9
E	-7	HIS	-	expression tag	UNP Q5ZVV9
E	-6	HIS	-	expression tag	UNP Q5ZVV9
E	-5	HIS	-	expression tag	UNP Q5ZVV9
E	-4	HIS	-	expression tag	UNP Q5ZVV9
E	-3	HIS	-	expression tag	UNP Q5ZVV9
E	-2	HIS	-	expression tag	UNP Q5ZVV9
E	-1	GLY	-	expression tag	UNP Q5ZVV9
E	0	SER	-	expression tag	UNP Q5ZVV9
E	190	ALA	SER	engineered mutation	UNP Q5ZVV9
F	-11	MET	-	initiating methionine	UNP Q5ZVV9
F	-10	ARG	-	expression tag	UNP Q5ZVV9
F	-9	GLY	-	expression tag	UNP Q5ZVV9
F	-8	SER	-	expression tag	UNP Q5ZVV9
F	-7	HIS	-	expression tag	UNP Q5ZVV9
F	-6	HIS	-	expression tag	UNP Q5ZVV9
F	-5	HIS	-	expression tag	UNP Q5ZVV9
F	-4	HIS	-	expression tag	UNP Q5ZVV9
F	-3	HIS	-	expression tag	UNP Q5ZVV9
F	-2	HIS	-	expression tag	UNP Q5ZVV9
F	-1	GLY	-	expression tag	UNP Q5ZVV9
F	0	SER	-	expression tag	UNP Q5ZVV9
F	190	ALA	SER	engineered mutation	UNP Q5ZVV9
G	-11	MET	-	initiating methionine	UNP Q5ZVV9
G	-10	ARG	-	expression tag	UNP Q5ZVV9
G	-9	GLY	-	expression tag	UNP Q5ZVV9
G	-8	SER	-	expression tag	UNP Q5ZVV9
G	-7	HIS	-	expression tag	UNP Q5ZVV9
G	-6	HIS	-	expression tag	UNP Q5ZVV9
G	-5	HIS	-	expression tag	UNP Q5ZVV9
G	-4	HIS	-	expression tag	UNP Q5ZVV9
G	-3	HIS	-	expression tag	UNP Q5ZVV9
G	-2	HIS	-	expression tag	UNP Q5ZVV9
G	-1	GLY	-	expression tag	UNP Q5ZVV9
G	0	SER	-	expression tag	UNP Q5ZVV9
G	190	ALA	SER	engineered mutation	UNP Q5ZVV9
H	-11	MET	-	initiating methionine	UNP Q5ZVV9
H	-10	ARG	-	expression tag	UNP Q5ZVV9
H	-9	GLY	-	expression tag	UNP Q5ZVV9
H	-8	SER	-	expression tag	UNP Q5ZVV9
H	-7	HIS	-	expression tag	UNP Q5ZVV9
H	-6	HIS	-	expression tag	UNP Q5ZVV9

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-5	HIS	-	expression tag	UNP Q5ZVV9
H	-4	HIS	-	expression tag	UNP Q5ZVV9
H	-3	HIS	-	expression tag	UNP Q5ZVV9
H	-2	HIS	-	expression tag	UNP Q5ZVV9
H	-1	GLY	-	expression tag	UNP Q5ZVV9
H	0	SER	-	expression tag	UNP Q5ZVV9
H	190	ALA	SER	engineered mutation	UNP Q5ZVV9

- Molecule 2 is a protein called Octapeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	8	Total	C	N	O	0	0	0
			40	24	8	8			

- Molecule 3 is a protein called Hexa-peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	J	6	Total	C	N	O	0	0	0
			30	18	6	6			
3	L	6	Total	C	N	O	0	0	0
			30	18	6	6			

- Molecule 4 is a protein called Hepta-peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	K	7	Total	C	N	O	0	0	0
			35	21	7	7			
4	M	7	Total	C	N	O	0	0	0
			35	21	7	7			
4	N	7	Total	C	N	O	0	0	0
			35	21	7	7			
4	O	7	Total	C	N	O	0	0	0
			35	21	7	7			
4	P	7	Total	C	N	O	0	0	0
			35	21	7	7			

- Molecule 5 is a protein called UNK-UNK-UNK.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	Q	3	Total	C	N	O	0	0	0
			16	9	3	4			

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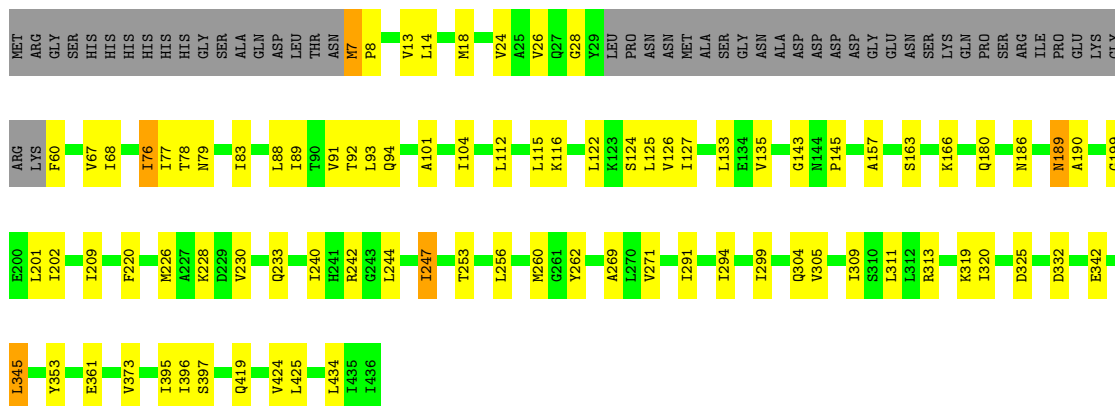
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	R	3	Total	C	N	O	0	0	0
			16	9	3	4			
5	S	3	Total	C	N	O	0	0	0
			16	9	3	4			
5	T	3	Total	C	N	O	0	0	0
			16	9	3	4			
5	U	3	Total	C	N	O	0	0	0
			16	9	3	4			
5	V	3	Total	C	N	O	0	0	0
			16	9	3	4			

3 Residue-property plots

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.

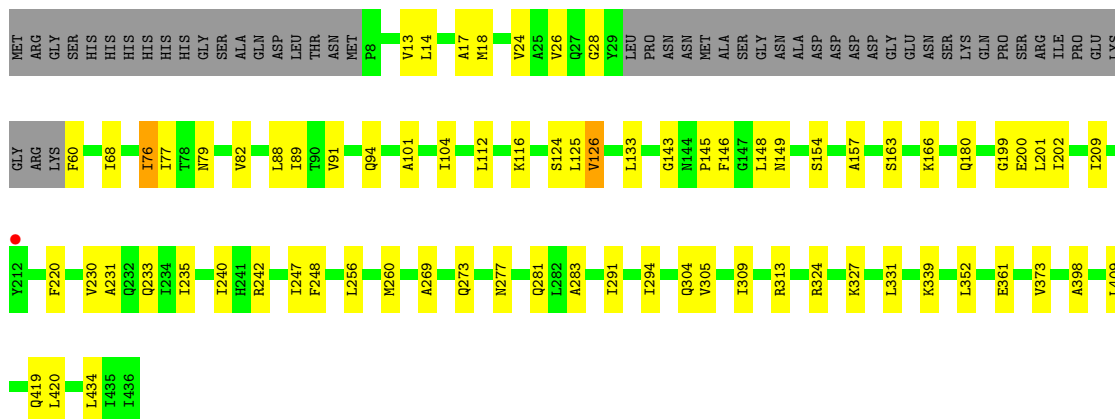
• Molecule 1: Protease DO

Chain A: 



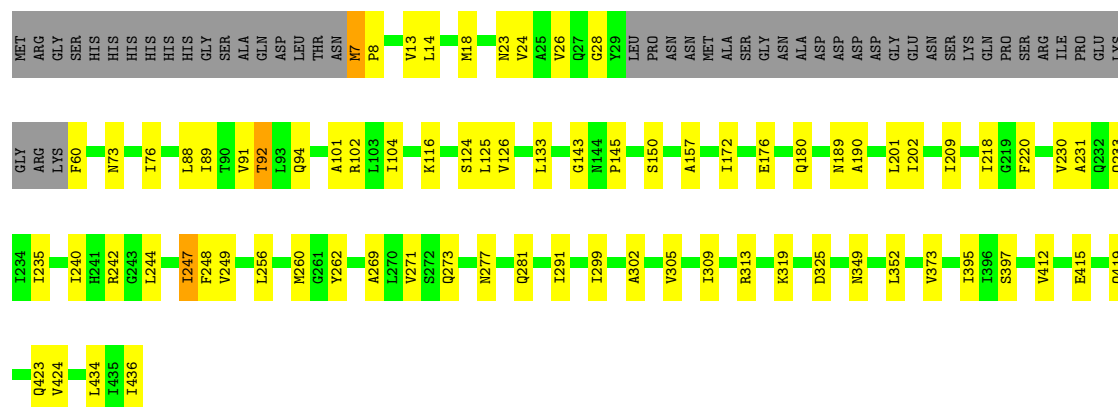
• Molecule 1: Protease DO

Chain B: 



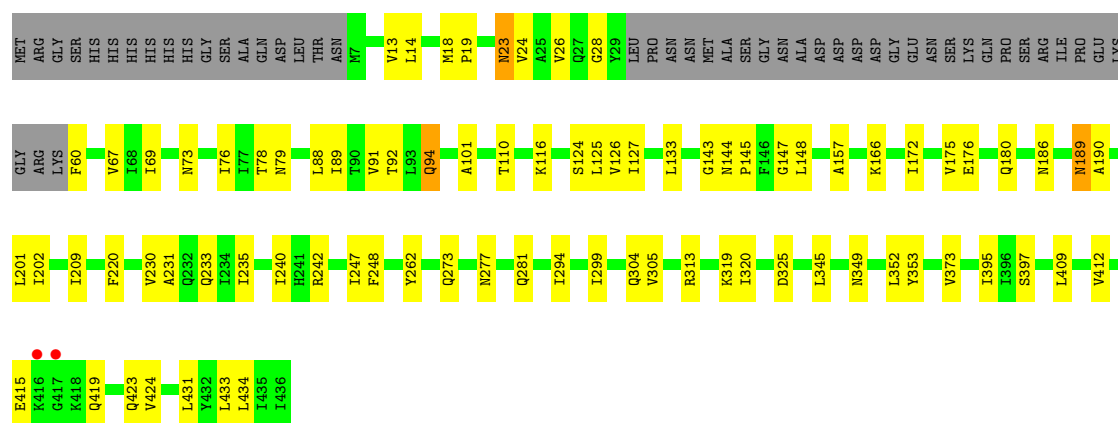
• Molecule 1: Protease DO

Chain C: 



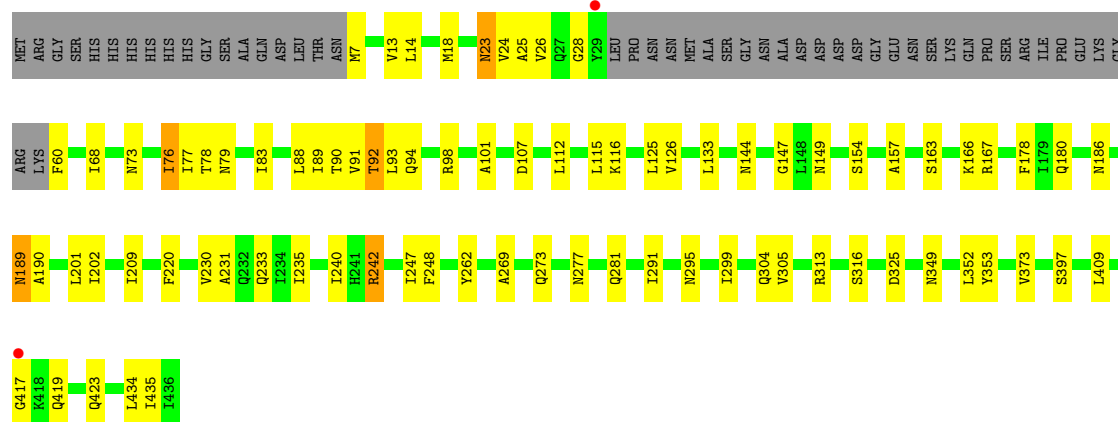
• Molecule 1: Protease DO

Chain D: 71% 18% 11%



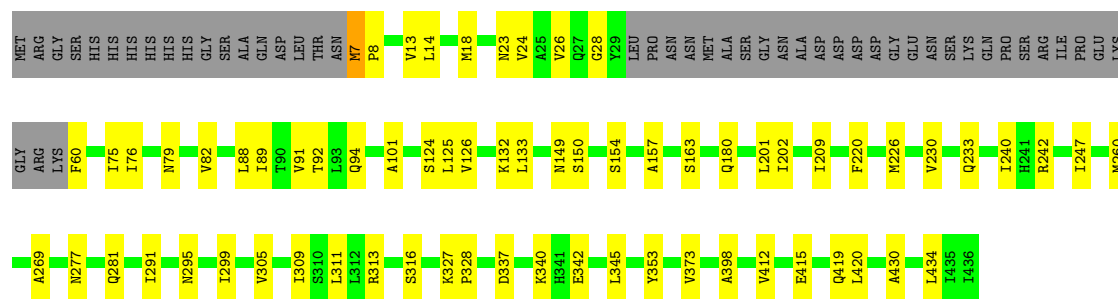
• Molecule 1: Protease DO

Chain E: 71% 17% 11%



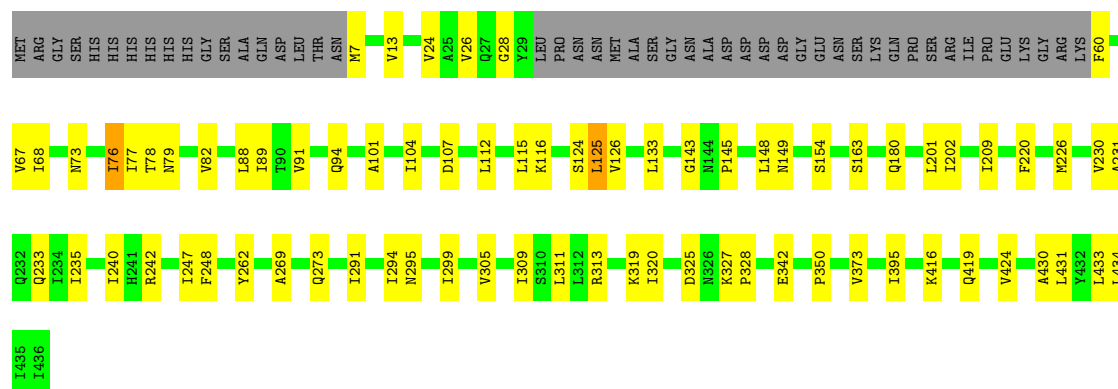
• Molecule 1: Protease DO

Chain F: 74% 15% 11%



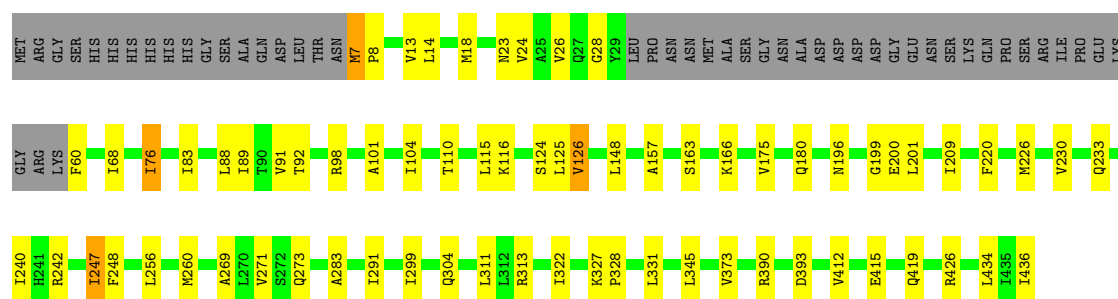
- Molecule 1: Protease DO

Chain G: 73% 16% 11%



- Molecule 1: Protease DO

Chain H: 74% 15% 11%



- Molecule 2: Octapeptide

Chain I: 88% 12%



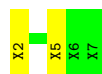
- Molecule 3: Hexa-peptide

Chain J: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: Hexa-peptide

Chain L:  67% 33%



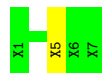
- Molecule 4: Hepta-peptide

Chain K:  86% 14%

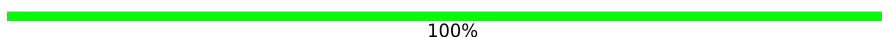


- Molecule 4: Hepta-peptide

Chain M:  86% 14%

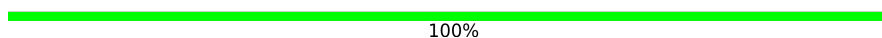


- Molecule 4: Hepta-peptide

Chain N:  100%

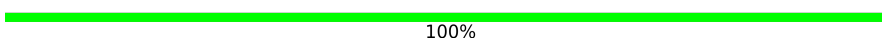
There are no outlier residues recorded for this chain.

- Molecule 4: Hepta-peptide

Chain O:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: Hepta-peptide

Chain P:  100%

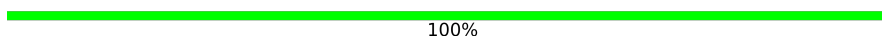
There are no outlier residues recorded for this chain.

- Molecule 5: UNK-UNK-UNK

Chain Q:  67% 33%



- Molecule 5: UNK-UNK-UNK

Chain R:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: UNK-UNK-UNK

Chain S:  67% 33%

X105
X106
X107

- Molecule 5: UNK-UNK-UNK

Chain T:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: UNK-UNK-UNK

Chain U:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: UNK-UNK-UNK

Chain V:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	147.91Å 147.91Å 383.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.54 – 3.20 28.54 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (28.54-3.20) 98.9 (28.54-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.17Å)	Xtriage
Refinement program	PHENIX 1.8.1 _1168	Depositor
R, R_{free}	0.181 , 0.219 0.185 , 0.221	Depositor DCC
R_{free} test set	3875 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	72.1	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.066 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24195	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.53% 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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.33	0/3018	0.79	2/4089 (0.0%)
1	B	0.34	0/3010	0.79	0/4078
1	C	0.34	0/3018	0.80	2/4089 (0.0%)
1	D	0.33	0/3018	0.78	0/4089
1	E	0.34	0/3018	0.80	5/4089 (0.1%)
1	F	0.33	0/3018	0.79	3/4089 (0.1%)
1	G	0.33	0/3018	0.78	3/4089 (0.1%)
1	H	0.33	0/3018	0.79	2/4089 (0.0%)
All	All	0.33	0/24136	0.79	17/32701 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	7	MET	CA-C-N	5.95	127.28	119.84
1	H	7	MET	C-N-CA	5.95	127.28	119.84
1	E	7	MET	CA-C-N	5.83	127.13	119.84
1	E	7	MET	C-N-CA	5.83	127.13	119.84
1	A	7	MET	CA-C-N	5.62	126.86	119.84
1	A	7	MET	C-N-CA	5.62	126.86	119.84
1	E	417	GLY	N-CA-C	-5.61	102.95	111.14
1	F	295	ASN	CB-CA-C	-5.54	110.21	116.63
1	G	7	MET	CA-C-N	5.42	126.61	119.84
1	G	7	MET	C-N-CA	5.42	126.61	119.84
1	E	295	ASN	CB-CA-C	-5.39	110.38	116.63
1	C	7	MET	CA-C-N	5.36	126.55	119.84
1	C	7	MET	C-N-CA	5.36	126.55	119.84
1	G	295	ASN	CB-CA-C	-5.36	110.42	116.63
1	F	7	MET	CA-C-N	5.29	126.46	119.84
1	F	7	MET	C-N-CA	5.29	126.46	119.84
1	E	435	ILE	N-CA-C	5.04	115.60	107.73

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2979	0	3088	50	0
1	B	2971	0	3080	42	0
1	C	2979	0	3088	46	0
1	D	2979	0	3088	47	0
1	E	2979	0	3088	47	0
1	F	2979	0	3088	36	0
1	G	2979	0	3088	41	0
1	H	2979	0	3088	44	0
2	I	40	0	11	1	0
3	J	30	0	8	0	0
3	L	30	0	8	2	0
4	K	35	0	9	1	0
4	M	35	0	9	1	0
4	N	35	0	9	0	0
4	O	35	0	9	0	0
4	P	35	0	9	0	0
5	Q	16	0	5	1	0
5	R	16	0	5	0	0
5	S	16	0	6	1	0
5	T	16	0	5	0	0
5	U	16	0	5	0	0
5	V	16	0	5	0	0
All	All	24195	0	24799	345	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (345) 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:E:125:LEU:HD11	1:E:201:LEU:HB2	1.58	0.85
1:D:23:ASN:HD21	1:D:144:ASN:HD22	1.25	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:VAL:HG13	1:D:240:ILE:HD11	1.67	0.77
1:D:125:LEU:HD11	1:D:201:LEU:HB2	1.66	0.75
1:B:230:VAL:HG13	1:B:240:ILE:HD11	1.69	0.72
1:E:209:ILE:HG13	1:E:220:PHE:HE2	1.55	0.72
1:H:230:VAL:HG13	1:H:240:ILE:HD11	1.71	0.71
1:A:230:VAL:HG13	1:A:240:ILE:HD11	1.71	0.71
1:G:230:VAL:HG13	1:G:240:ILE:HD11	1.73	0.71
1:B:89:ILE:HG13	1:B:101:ALA:HB3	1.73	0.70
1:C:209:ILE:HG13	1:C:220:PHE:HE2	1.57	0.70
1:F:230:VAL:HG13	1:F:240:ILE:HD11	1.74	0.69
1:F:18:MET:HE1	1:F:157:ALA:HB2	1.75	0.69
1:A:24:VAL:HG12	1:A:91:VAL:HG22	1.74	0.68
1:C:24:VAL:HG12	1:C:91:VAL:HG22	1.75	0.68
1:B:18:MET:HE1	1:B:157:ALA:HB2	1.76	0.67
1:D:209:ILE:HG13	1:D:220:PHE:HE2	1.58	0.67
1:D:89:ILE:HG13	1:D:101:ALA:HB3	1.77	0.66
1:B:209:ILE:HG13	1:B:220:PHE:HE2	1.59	0.66
1:E:230:VAL:HG13	1:E:240:ILE:HD11	1.77	0.66
1:C:26:VAL:HG22	1:C:89:ILE:HG22	1.78	0.66
1:D:23:ASN:HD21	1:D:144:ASN:ND2	1.94	0.65
1:C:230:VAL:HG13	1:C:240:ILE:HD11	1.80	0.64
1:C:18:MET:HE1	1:C:157:ALA:HB2	1.78	0.64
1:C:23:ASN:HB2	1:C:92:THR:HG23	1.79	0.64
1:A:89:ILE:HG13	1:A:101:ALA:HB3	1.79	0.64
1:E:26:VAL:HG22	1:E:89:ILE:HG22	1.78	0.64
1:B:233:GLN:HE21	1:B:313:ARG:HH11	1.46	0.64
1:G:26:VAL:HG22	1:G:89:ILE:HG22	1.80	0.64
1:H:89:ILE:HG13	1:H:101:ALA:HB3	1.79	0.64
1:E:25:ALA:HB3	1:E:90:THR:HG23	1.80	0.63
1:F:233:GLN:HE21	1:F:313:ARG:HH11	1.46	0.63
1:B:26:VAL:HG22	1:B:89:ILE:HG22	1.80	0.63
1:A:233:GLN:HE21	1:A:313:ARG:HH11	1.46	0.62
1:D:26:VAL:HG22	1:D:89:ILE:HG22	1.82	0.62
1:B:324:ARG:O	1:B:327:LYS:HG2	2.00	0.62
1:D:419:GLN:HG3	1:D:434:LEU:HD11	1.81	0.61
1:E:18:MET:HE1	1:E:157:ALA:HB2	1.83	0.61
1:F:125:LEU:HD11	1:F:201:LEU:HB2	1.82	0.61
1:A:209:ILE:HG13	1:A:220:PHE:HE2	1.64	0.61
1:A:269:ALA:HB3	1:A:291:ILE:HB	1.81	0.61
1:C:233:GLN:HE21	1:C:313:ARG:HH11	1.47	0.61
1:D:233:GLN:HE21	1:D:313:ARG:HH11	1.46	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:107:ASP:OD2	1:G:242:ARG:NH2	2.33	0.60
1:E:23:ASN:HD21	1:E:144:ASN:HD22	1.48	0.60
1:G:68:ILE:HG12	1:G:76:ILE:HG22	1.83	0.60
1:E:23:ASN:HD21	1:E:144:ASN:ND2	1.99	0.59
1:F:299:ILE:HD13	1:F:305:VAL:HG22	1.83	0.59
1:A:127:ILE:HG21	1:A:228:LYS:HE2	1.84	0.59
1:D:277:ASN:N	1:D:281:GLN:OE1	2.34	0.59
1:G:89:ILE:HG13	1:G:101:ALA:HB3	1.84	0.59
1:H:26:VAL:HG22	1:H:89:ILE:HG22	1.84	0.59
1:A:419:GLN:HG3	1:A:434:LEU:HD11	1.85	0.58
1:G:209:ILE:HG13	1:G:220:PHE:HE2	1.67	0.58
1:C:125:LEU:HD11	1:C:201:LEU:HB2	1.85	0.58
1:F:209:ILE:HG13	1:F:220:PHE:HE2	1.67	0.58
1:D:397:SER:HB3	1:D:423:GLN:HB3	1.86	0.58
1:A:332:ASP:OD2	1:C:102:ARG:NH2	2.36	0.58
1:F:89:ILE:HG13	1:F:101:ALA:HB3	1.85	0.58
1:E:68:ILE:HG12	1:E:76:ILE:HG22	1.84	0.58
1:B:28:GLY:O	1:B:60:PHE:HB3	2.04	0.58
1:C:419:GLN:HG3	1:C:434:LEU:HD11	1.86	0.57
1:H:233:GLN:HE21	1:H:313:ARG:HH11	1.51	0.57
1:A:18:MET:HE1	1:A:157:ALA:HB2	1.85	0.57
1:E:89:ILE:HG13	1:E:101:ALA:HB3	1.85	0.57
1:G:24:VAL:HG12	1:G:91:VAL:HG22	1.86	0.57
1:G:431:LEU:HD23	1:G:433:LEU:HD21	1.87	0.57
1:H:419:GLN:HG3	1:H:434:LEU:HD11	1.86	0.57
1:C:248:PHE:HB2	1:C:273:GLN:HB3	1.86	0.57
1:E:233:GLN:HE21	1:E:313:ARG:HH11	1.52	0.56
1:F:24:VAL:HG12	1:F:91:VAL:HG22	1.85	0.56
1:B:419:GLN:HG3	1:B:434:LEU:HD11	1.87	0.56
1:D:125:LEU:CD1	1:D:201:LEU:HB2	2.35	0.56
1:G:419:GLN:HG3	1:G:434:LEU:HD11	1.85	0.56
1:H:125:LEU:HD11	1:H:199:GLY:O	2.04	0.56
1:H:269:ALA:HB3	1:H:291:ILE:HB	1.85	0.56
1:H:24:VAL:HG12	1:H:91:VAL:HG22	1.86	0.56
1:C:14:LEU:O	1:C:18:MET:HG2	2.06	0.56
1:A:14:LEU:O	1:A:18:MET:HG2	2.06	0.56
1:F:26:VAL:HG22	1:F:89:ILE:HG22	1.86	0.56
1:D:18:MET:HE1	1:D:157:ALA:HB2	1.87	0.56
1:E:269:ALA:HB3	1:E:291:ILE:HB	1.88	0.56
1:H:14:LEU:HB3	1:H:18:MET:HE3	1.88	0.56
1:H:209:ILE:HG13	1:H:220:PHE:HE2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:419:GLN:HG3	1:E:434:LEU:HD11	1.87	0.55
1:E:28:GLY:O	1:E:60:PHE:HB3	2.07	0.55
1:B:256:LEU:O	1:B:260:MET:HG3	2.07	0.55
1:D:262:TYR:OH	1:D:325:ASP:O	2.23	0.55
1:G:233:GLN:HE21	1:G:313:ARG:HH11	1.55	0.55
1:G:133:LEU:HD11	1:G:202:ILE:HD12	1.89	0.54
1:C:89:ILE:HG13	1:C:101:ALA:HB3	1.88	0.54
1:E:24:VAL:HG12	1:E:91:VAL:HG22	1.88	0.54
1:F:419:GLN:HG3	1:F:434:LEU:HD11	1.89	0.54
1:A:124:SER:OG	1:A:125:LEU:N	2.40	0.54
1:D:24:VAL:HG12	1:D:91:VAL:HG22	1.88	0.54
1:C:277:ASN:N	1:C:281:GLN:OE1	2.37	0.54
1:A:247:ILE:HD11	1:A:271:VAL:HG22	1.90	0.54
1:B:124:SER:OG	1:B:125:LEU:N	2.40	0.54
1:C:28:GLY:O	1:C:60:PHE:HB3	2.07	0.54
1:F:125:LEU:CD1	1:F:201:LEU:HB2	2.38	0.54
1:C:125:LEU:CD1	1:C:201:LEU:HB2	2.38	0.54
1:B:269:ALA:HB3	1:B:291:ILE:HB	1.90	0.54
1:G:76:ILE:HD11	1:G:115:LEU:HD12	1.90	0.54
1:H:110:THR:HG22	1:H:175:VAL:HB	1.90	0.54
1:B:133:LEU:HD11	1:B:202:ILE:HD12	1.90	0.53
1:C:180:GLN:HG3	1:C:220:PHE:CE1	2.43	0.53
1:G:269:ALA:HB3	1:G:291:ILE:HB	1.90	0.53
1:C:133:LEU:HD11	1:C:202:ILE:HD12	1.91	0.52
1:H:166:LYS:HE3	1:H:304:GLN:HE21	1.74	0.52
1:B:14:LEU:O	1:B:18:MET:HG2	2.09	0.52
1:B:248:PHE:HB2	1:B:273:GLN:HB3	1.91	0.52
1:C:256:LEU:O	1:C:260:MET:HG3	2.10	0.52
1:F:342:GLU:OE1	1:F:353:TYR:OH	2.27	0.52
1:A:135:VAL:HG11	1:H:18:MET:HE1	1.91	0.52
1:D:14:LEU:O	1:D:18:MET:HG2	2.10	0.52
1:E:397:SER:HB3	1:E:423:GLN:HB3	1.92	0.52
1:H:28:GLY:O	1:H:60:PHE:HB3	2.10	0.52
1:G:124:SER:OG	1:G:125:LEU:N	2.43	0.52
1:D:69:ILE:HG23	1:D:127:ILE:HD11	1.91	0.51
1:H:180:GLN:HG3	1:H:220:PHE:CE1	2.46	0.51
1:F:277:ASN:N	1:F:281:GLN:OE1	2.41	0.51
1:D:28:GLY:O	1:D:60:PHE:HB3	2.11	0.51
1:F:313:ARG:O	1:F:316:SER:OG	2.27	0.51
1:E:73:ASN:O	1:E:116:LYS:HE3	2.10	0.51
1:E:125:LEU:CD1	1:E:201:LEU:HB2	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:180:GLN:HG3	1:F:220:PHE:CE1	2.46	0.51
1:B:125:LEU:HD11	1:B:199:GLY:O	2.11	0.51
1:A:190:ALA:HB2	2:I:5:UNK:O	2.10	0.51
1:A:93:LEU:HD21	1:A:122:LEU:HD23	1.94	0.50
1:F:28:GLY:O	1:F:60:PHE:HB3	2.10	0.50
1:C:397:SER:HB3	1:C:423:GLN:HB3	1.93	0.50
1:G:233:GLN:NE2	1:G:313:ARG:HG3	2.26	0.50
1:A:26:VAL:HG22	1:A:89:ILE:HG22	1.93	0.50
1:B:180:GLN:HG3	1:B:220:PHE:CE1	2.47	0.50
1:A:233:GLN:HE21	1:A:313:ARG:NH1	2.10	0.50
1:E:186:ASN:O	1:E:189:ASN:HB2	2.12	0.50
1:F:269:ALA:HB3	1:F:291:ILE:HB	1.92	0.50
1:H:124:SER:OG	1:H:125:LEU:N	2.44	0.50
1:C:269:ALA:HB3	1:C:291:ILE:HB	1.93	0.50
1:A:28:GLY:O	1:A:60:PHE:HB3	2.12	0.49
1:A:125:LEU:HD23	1:A:201:LEU:HB2	1.93	0.49
1:F:14:LEU:O	1:F:18:MET:HG2	2.12	0.49
1:A:125:LEU:HD11	1:A:199:GLY:O	2.12	0.49
1:C:262:TYR:OH	1:C:325:ASP:O	2.23	0.49
1:D:23:ASN:ND2	1:D:144:ASN:HD22	2.01	0.49
1:A:166:LYS:HE3	1:A:304:GLN:HE21	1.78	0.49
1:A:104:ILE:HD11	1:A:116:LYS:HB2	1.93	0.49
1:F:23:ASN:HB2	1:F:92:THR:HB	1.94	0.49
1:G:76:ILE:HG13	1:G:115:LEU:HB2	1.95	0.49
1:C:172:ILE:N	1:C:176:GLU:OE1	2.46	0.48
1:A:332:ASP:OD2	1:C:116:LYS:HD3	2.13	0.48
1:C:247:ILE:HD11	1:C:271:VAL:HG22	1.94	0.48
1:A:262:TYR:OH	1:A:325:ASP:O	2.29	0.48
1:H:104:ILE:HD11	1:H:116:LYS:HB2	1.94	0.48
1:A:226:MET:HG3	1:A:311:LEU:HD11	1.94	0.48
1:E:262:TYR:OH	1:E:325:ASP:O	2.28	0.48
1:B:233:GLN:HE21	1:B:313:ARG:NH1	2.11	0.48
1:E:166:LYS:HE3	1:E:304:GLN:HE21	1.78	0.48
1:E:231:ALA:O	1:E:235:ILE:HG13	2.13	0.48
1:D:395:ILE:HG12	1:D:424:VAL:HG12	1.95	0.48
1:E:107:ASP:OD2	1:E:242:ARG:NH2	2.46	0.48
1:C:273:GLN:HB2	1:F:430:ALA:HB3	1.95	0.48
1:D:248:PHE:HB2	1:D:273:GLN:HB3	1.96	0.48
1:E:14:LEU:O	1:E:18:MET:HG2	2.14	0.48
1:E:83:ILE:HD13	1:E:115:LEU:HD21	1.96	0.48
1:B:68:ILE:HG12	1:B:76:ILE:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:LYS:HE3	1:B:304:GLN:HE21	1.79	0.47
1:H:226:MET:HG3	1:H:311:LEU:HD11	1.95	0.47
1:A:244:LEU:HG	5:Q:107:UNK:OXT	2.13	0.47
1:E:180:GLN:HG3	1:E:220:PHE:CE1	2.50	0.47
1:D:110:THR:HG22	1:D:175:VAL:HB	1.96	0.47
1:H:68:ILE:HG12	1:H:76:ILE:HG22	1.97	0.47
1:A:68:ILE:HG12	1:A:76:ILE:HG22	1.97	0.47
1:G:77:ILE:HD11	1:G:112:LEU:HD22	1.96	0.47
1:A:133:LEU:HD11	1:A:202:ILE:HD12	1.96	0.47
1:C:231:ALA:O	1:C:235:ILE:HG13	2.15	0.47
1:C:299:ILE:HD13	1:C:305:VAL:HG22	1.97	0.47
1:C:349:ASN:HD21	1:C:352:LEU:HB2	1.80	0.47
1:G:180:GLN:HG3	1:G:220:PHE:CE1	2.49	0.47
1:D:78:THR:OG1	1:D:79:ASN:N	2.48	0.47
1:D:209:ILE:HA	3:L:2:UNK:HA	1.97	0.47
1:D:299:ILE:HD13	1:D:305:VAL:HG22	1.97	0.47
1:E:277:ASN:N	1:E:281:GLN:OE1	2.43	0.47
1:C:14:LEU:HB3	1:C:18:MET:HE2	1.97	0.47
1:B:277:ASN:N	1:B:281:GLN:OE1	2.45	0.47
1:C:124:SER:OG	1:C:125:LEU:N	2.48	0.47
1:A:395:ILE:HG12	1:A:424:VAL:HG12	1.97	0.46
1:G:67:VAL:HG11	1:G:201:LEU:HD22	1.97	0.46
1:C:233:GLN:HE21	1:C:313:ARG:NH1	2.13	0.46
1:D:186:ASN:O	1:D:189:ASN:HB2	2.16	0.46
1:G:350:PRO:HG3	1:G:416:LYS:HE2	1.96	0.46
1:E:163:SER:N	1:E:180:GLN:O	2.48	0.46
1:C:190:ALA:HB2	4:K:5:UNK:O	2.16	0.45
1:C:395:ILE:HG12	1:C:424:VAL:HG12	1.98	0.45
1:A:253:THR:HG21	1:H:98:ARG:HH12	1.80	0.45
1:A:7:MET:HA	1:A:8:PRO:HD3	1.75	0.45
1:A:67:VAL:HG11	1:A:201:LEU:HD22	1.98	0.45
1:H:196:ASN:OD1	1:H:200:GLU:N	2.49	0.45
1:H:256:LEU:O	1:H:260:MET:HG3	2.17	0.45
1:E:313:ARG:O	1:E:316:SER:OG	2.30	0.45
1:G:430:ALA:HB3	1:H:273:GLN:HB2	1.97	0.45
1:H:248:PHE:HB2	1:H:273:GLN:HB3	1.97	0.45
1:H:412:VAL:O	1:H:415:GLU:HG2	2.16	0.45
1:C:104:ILE:HD11	1:C:116:LYS:HB2	1.98	0.45
1:C:244:LEU:HG	5:S:107:UNK:OXT	2.17	0.45
1:D:133:LEU:HD11	1:D:202:ILE:HD12	1.99	0.45
1:E:233:GLN:NE2	1:E:240:ILE:HG23	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:352:LEU:HD11	1:D:409:LEU:HG	1.99	0.45
1:B:163:SER:N	1:B:180:GLN:O	2.47	0.45
1:G:262:TYR:OH	1:G:325:ASP:O	2.31	0.45
1:H:76:ILE:HD11	1:H:115:LEU:HD12	1.99	0.45
1:E:76:ILE:HG13	1:E:115:LEU:HB2	1.98	0.45
1:B:104:ILE:HD11	1:B:116:LYS:HB2	1.99	0.44
1:D:19:PRO:HA	1:D:94:GLN:HG2	2.00	0.44
1:G:248:PHE:HB2	1:G:273:GLN:HB3	1.99	0.44
1:G:299:ILE:HD13	1:G:305:VAL:HG22	1.99	0.44
1:B:233:GLN:NE2	1:B:240:ILE:HG23	2.32	0.44
1:D:209:ILE:HG13	1:D:220:PHE:CE2	2.45	0.44
1:E:233:GLN:HE21	1:E:313:ARG:NH1	2.15	0.44
1:C:305:VAL:O	1:C:309:ILE:HG12	2.18	0.44
1:E:92:THR:HB	1:E:98:ARG:HG2	1.99	0.44
1:B:126:VAL:HG13	1:B:200:GLU:HA	1.99	0.44
1:E:23:ASN:ND2	1:E:144:ASN:HD22	2.14	0.44
1:A:256:LEU:O	1:A:260:MET:HG3	2.18	0.44
1:D:294:ILE:HG12	1:D:320:ILE:HD12	1.99	0.44
1:A:186:ASN:O	1:A:189:ASN:HB2	2.17	0.44
1:B:352:LEU:HD11	1:B:409:LEU:HG	2.00	0.44
1:F:233:GLN:HE21	1:F:313:ARG:NH1	2.14	0.44
1:G:163:SER:N	1:G:180:GLN:O	2.51	0.44
1:A:299:ILE:HD13	1:A:305:VAL:HG22	2.00	0.44
1:B:14:LEU:HB3	1:B:18:MET:HE2	1.99	0.44
1:B:231:ALA:O	1:B:235:ILE:HG13	2.17	0.44
1:B:146:PHE:CD2	1:C:218:ILE:HD12	2.52	0.43
1:C:319:LYS:HB2	1:C:319:LYS:HE3	1.86	0.43
1:G:104:ILE:HD11	1:G:116:LYS:HB2	2.00	0.43
1:H:393:ASP:OD2	1:H:426:ARG:NH2	2.38	0.43
1:A:180:GLN:HG3	1:A:220:PHE:CE1	2.53	0.43
1:C:143:GLY:O	1:C:145:PRO:HD3	2.18	0.43
1:E:144:ASN:HD21	1:E:147:GLY:HA2	1.83	0.43
1:H:126:VAL:HG13	1:H:200:GLU:HA	1.99	0.43
1:H:163:SER:N	1:H:180:GLN:O	2.48	0.43
1:B:305:VAL:O	1:B:309:ILE:HG12	2.19	0.43
1:B:294:ILE:HD13	1:B:309:ILE:HD11	1.99	0.43
1:G:294:ILE:HG12	1:G:320:ILE:HD12	2.00	0.43
1:A:163:SER:N	1:A:180:GLN:O	2.49	0.43
1:H:23:ASN:HB2	1:H:92:THR:HB	2.00	0.43
1:H:247:ILE:HD11	1:H:271:VAL:HG22	2.00	0.43
1:G:73:ASN:O	1:G:116:LYS:HE3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:283:ALA:O	1:H:331:LEU:HD22	2.19	0.43
1:A:77:ILE:HD11	1:A:112:LEU:HD22	2.00	0.43
1:H:125:LEU:HD23	1:H:201:LEU:HB2	2.01	0.43
1:F:398:ALA:HB1	1:F:420:LEU:HD11	2.00	0.43
1:E:352:LEU:HD11	1:E:409:LEU:HG	2.01	0.42
1:H:83:ILE:HD13	1:H:115:LEU:HD21	2.01	0.42
1:A:14:LEU:HB3	1:A:18:MET:HE2	2.00	0.42
1:E:78:THR:OG1	1:E:79:ASN:N	2.51	0.42
1:F:133:LEU:HD11	1:F:202:ILE:HD12	2.02	0.42
1:H:148:LEU:HD23	1:H:148:LEU:HA	1.85	0.42
1:D:180:GLN:HG3	1:D:220:PHE:CE1	2.54	0.42
1:D:190:ALA:HB2	3:L:5:UNK:O	2.20	0.42
1:D:412:VAL:O	1:D:415:GLU:HG2	2.19	0.42
1:E:133:LEU:HD11	1:E:202:ILE:HD12	2.01	0.42
1:E:299:ILE:HD13	1:E:305:VAL:HG22	2.01	0.42
1:G:28:GLY:O	1:G:60:PHE:HB3	2.18	0.42
1:G:319:LYS:HB2	1:G:319:LYS:HE3	1.89	0.42
1:A:319:LYS:HB2	1:A:319:LYS:HE3	1.89	0.42
1:A:345:LEU:HD12	1:A:345:LEU:HA	1.84	0.42
1:B:125:LEU:HD23	1:B:201:LEU:HB2	2.01	0.42
1:E:149:ASN:HB3	1:E:154:SER:O	2.20	0.42
1:G:294:ILE:HD13	1:G:309:ILE:HD11	2.02	0.42
1:F:124:SER:OG	1:F:125:LEU:N	2.53	0.42
1:B:143:GLY:O	1:B:145:PRO:HD3	2.19	0.42
1:C:209:ILE:HG13	1:C:220:PHE:CE2	2.47	0.42
1:D:124:SER:OG	1:D:125:LEU:N	2.53	0.42
1:G:79:ASN:HB2	1:G:82:VAL:HG23	2.01	0.42
1:B:233:GLN:NE2	1:B:313:ARG:HG3	2.34	0.42
1:C:233:GLN:NE2	1:C:313:ARG:HG3	2.35	0.42
1:G:231:ALA:O	1:G:235:ILE:HG13	2.19	0.42
1:C:412:VAL:O	1:C:415:GLU:HG2	2.20	0.42
1:D:349:ASN:O	1:D:353:TYR:HB2	2.20	0.42
1:B:24:VAL:HG12	1:B:91:VAL:HG22	2.01	0.42
1:F:337:ASP:HB3	1:F:340:LYS:HB3	2.02	0.42
1:B:79:ASN:HB2	1:B:82:VAL:HG23	2.01	0.42
1:A:78:THR:OG1	1:A:79:ASN:N	2.53	0.41
1:A:294:ILE:HG12	1:A:320:ILE:HD12	2.02	0.41
1:B:283:ALA:O	1:B:331:LEU:HD22	2.20	0.41
1:F:7:MET:HA	1:F:8:PRO:HD3	1.77	0.41
1:C:7:MET:HA	1:C:8:PRO:HD3	1.76	0.41
1:D:431:LEU:HD23	1:D:433:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:148:LEU:HD23	1:G:148:LEU:HA	1.89	0.41
1:H:299:ILE:HA	1:H:304:GLN:OE1	2.20	0.41
1:A:143:GLY:O	1:A:145:PRO:HD3	2.20	0.41
1:C:73:ASN:O	1:C:116:LYS:HE3	2.20	0.41
1:D:148:LEU:HD23	1:D:148:LEU:HA	1.88	0.41
1:F:79:ASN:HB2	1:F:82:VAL:HG23	2.01	0.41
1:F:327:LYS:HA	1:F:328:PRO:HD3	1.87	0.41
1:H:18:MET:CE	1:H:157:ALA:HB2	2.50	0.41
1:D:166:LYS:HE3	1:D:304:GLN:HE21	1.85	0.41
1:E:248:PHE:HB2	1:E:273:GLN:HB3	2.02	0.41
1:H:233:GLN:HE21	1:H:313:ARG:NH1	2.16	0.41
1:F:163:SER:N	1:F:180:GLN:O	2.52	0.41
1:F:305:VAL:O	1:F:309:ILE:HG12	2.21	0.41
1:F:412:VAL:O	1:F:415:GLU:HG2	2.21	0.41
1:G:143:GLY:O	1:G:145:PRO:HD3	2.20	0.41
1:C:249:VAL:HG12	1:C:302:ALA:HB1	2.03	0.41
1:D:172:ILE:N	1:D:176:GLU:OE1	2.52	0.41
1:E:190:ALA:HB2	4:M:5:UNK:O	2.20	0.41
1:G:327:LYS:HA	1:G:328:PRO:HD3	1.90	0.41
1:E:167:ARG:HB2	1:E:178:PHE:HB2	2.03	0.41
1:F:133:LEU:HD11	1:F:202:ILE:HB	2.02	0.41
1:G:395:ILE:HG12	1:G:424:VAL:HG12	2.03	0.41
1:B:17:ALA:HA	1:B:125:LEU:HD13	2.03	0.41
1:B:77:ILE:HD11	1:B:112:LEU:HD22	2.03	0.41
1:D:231:ALA:O	1:D:235:ILE:HG13	2.20	0.41
1:D:319:LYS:HB2	1:D:319:LYS:HE3	1.86	0.41
1:E:77:ILE:HD11	1:E:112:LEU:HD22	2.03	0.41
1:F:149:ASN:HD22	1:F:154:SER:H	1.69	0.41
1:G:233:GLN:NE2	1:G:240:ILE:HG23	2.35	0.41
1:H:18:MET:HE2	1:H:157:ALA:HB2	2.03	0.41
1:A:342:GLU:OE2	1:A:353:TYR:OH	2.39	0.40
1:E:76:ILE:HD11	1:E:115:LEU:HD12	2.03	0.40
1:F:132:LYS:HD3	1:F:132:LYS:HA	1.89	0.40
1:A:83:ILE:HD13	1:A:115:LEU:HD21	2.03	0.40
1:A:396:ILE:HD13	1:A:425:LEU:HD11	2.03	0.40
1:E:144:ASN:ND2	1:E:147:GLY:HA2	2.36	0.40
1:F:226:MET:HG3	1:F:311:LEU:HD11	2.03	0.40
1:F:260:MET:HE2	1:F:260:MET:HB3	1.96	0.40
1:G:226:MET:HG3	1:G:311:LEU:HD11	2.03	0.40
1:B:149:ASN:HD22	1:B:154:SER:H	1.70	0.40
1:B:398:ALA:HB1	1:B:420:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:VAL:HG11	1:D:201:LEU:HD22	2.04	0.40
1:A:294:ILE:HD13	1:A:309:ILE:HD11	2.03	0.40
1:D:144:ASN:ND2	1:D:147:GLY:HA2	2.36	0.40
1:G:149:ASN:HB3	1:G:154:SER:O	2.22	0.40
1:H:7:MET:HA	1:H:8:PRO:HD3	1.73	0.40
1:H:291:ILE:HD13	1:H:322:ILE:HG22	2.03	0.40
1:H:327:LYS:HA	1:H:328:PRO:HD3	1.91	0.40
1:H:390:ARG:HD3	1:H:390:ARG:HA	1.90	0.40
1:A:135:VAL:CG1	1:H:18:MET:HE1	2.51	0.40
1:B:148:LEU:HD23	1:B:148:LEU:HA	1.87	0.40
1:D:73:ASN:O	1:D:116:LYS:HE3	2.21	0.40
1:D:143:GLY:O	1:D:145:PRO:HD3	2.21	0.40
1:D:233:GLN:NE2	1:D:313:ARG:HG3	2.36	0.40
1:E:349:ASN:O	1:E:353:TYR:HB2	2.20	0.40
1:G:78:THR:OG1	1:G:79:ASN:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	396/448 (88%)	388 (98%)	8 (2%)	0	100	100
1	B	395/448 (88%)	387 (98%)	8 (2%)	0	100	100
1	C	396/448 (88%)	387 (98%)	9 (2%)	0	100	100
1	D	396/448 (88%)	387 (98%)	9 (2%)	0	100	100
1	E	396/448 (88%)	388 (98%)	8 (2%)	0	100	100
1	F	396/448 (88%)	388 (98%)	8 (2%)	0	100	100
1	G	396/448 (88%)	389 (98%)	7 (2%)	0	100	100
1	H	396/448 (88%)	387 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3167/3584 (88%)	3101 (98%)	66 (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	322/362 (89%)	309 (96%)	13 (4%)	28	61
1	B	321/362 (89%)	311 (97%)	10 (3%)	35	66
1	C	322/362 (89%)	310 (96%)	12 (4%)	30	63
1	D	322/362 (89%)	310 (96%)	12 (4%)	30	63
1	E	322/362 (89%)	310 (96%)	12 (4%)	30	63
1	F	322/362 (89%)	311 (97%)	11 (3%)	32	64
1	G	322/362 (89%)	313 (97%)	9 (3%)	38	68
1	H	322/362 (89%)	313 (97%)	9 (3%)	38	68
All	All	2575/2896 (89%)	2487 (97%)	88 (3%)	32	64

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	76	ILE
1	A	88	LEU
1	A	92	THR
1	A	94	GLN
1	A	126	VAL
1	A	189	ASN
1	A	242	ARG
1	A	247	ILE
1	A	345	LEU
1	A	361	GLU
1	A	373	VAL

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Mol	Chain	Res	Type
1	A	397	SER
1	B	13	VAL
1	B	76	ILE
1	B	88	LEU
1	B	94	GLN
1	B	126	VAL
1	B	242	ARG
1	B	247	ILE
1	B	339	LYS
1	B	361	GLU
1	B	373	VAL
1	C	13	VAL
1	C	76	ILE
1	C	88	LEU
1	C	92	THR
1	C	94	GLN
1	C	126	VAL
1	C	150	SER
1	C	189	ASN
1	C	242	ARG
1	C	247	ILE
1	C	373	VAL
1	C	436	ILE
1	D	13	VAL
1	D	23	ASN
1	D	76	ILE
1	D	88	LEU
1	D	92	THR
1	D	94	GLN
1	D	126	VAL
1	D	189	ASN
1	D	242	ARG
1	D	247	ILE
1	D	345	LEU
1	D	373	VAL
1	E	13	VAL
1	E	23	ASN
1	E	76	ILE
1	E	88	LEU
1	E	92	THR
1	E	93	LEU
1	E	94	GLN

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Mol	Chain	Res	Type
1	E	126	VAL
1	E	189	ASN
1	E	242	ARG
1	E	247	ILE
1	E	373	VAL
1	F	13	VAL
1	F	75	ILE
1	F	76	ILE
1	F	88	LEU
1	F	94	GLN
1	F	126	VAL
1	F	150	SER
1	F	242	ARG
1	F	247	ILE
1	F	345	LEU
1	F	373	VAL
1	G	13	VAL
1	G	76	ILE
1	G	88	LEU
1	G	94	GLN
1	G	125	LEU
1	G	126	VAL
1	G	247	ILE
1	G	342	GLU
1	G	373	VAL
1	H	13	VAL
1	H	76	ILE
1	H	88	LEU
1	H	126	VAL
1	H	242	ARG
1	H	247	ILE
1	H	345	LEU
1	H	373	VAL
1	H	436	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	144	ASN
1	A	155	GLN
1	A	189	ASN

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Mol	Chain	Res	Type
1	A	233	GLN
1	A	251	HIS
1	A	374	GLN
1	B	23	ASN
1	B	144	ASN
1	B	155	GLN
1	B	233	GLN
1	B	326	ASN
1	B	374	GLN
1	C	189	ASN
1	C	233	GLN
1	C	251	HIS
1	C	326	ASN
1	C	341	HIS
1	D	23	ASN
1	D	155	GLN
1	D	233	GLN
1	D	251	HIS
1	D	326	ASN
1	D	374	GLN
1	E	144	ASN
1	E	155	GLN
1	E	233	GLN
1	E	258	GLN
1	E	293	GLN
1	E	374	GLN
1	F	233	GLN
1	G	233	GLN
1	G	293	GLN
1	G	374	GLN
1	H	149	ASN
1	H	205	ASN
1	H	233	GLN
1	H	251	HIS
1	H	258	GLN
1	H	273	GLN
1	H	326	ASN
1	H	374	GLN

5.3.3 RNA ⓘ

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	400/448 (89%)	-0.58	0 100 100	23, 58, 90, 112	0
1	B	399/448 (89%)	-0.52	1 (0%) 90 81	23, 51, 85, 112	0
1	C	400/448 (89%)	-0.57	0 100 100	22, 49, 81, 117	0
1	D	400/448 (89%)	-0.45	2 (0%) 87 76	25, 62, 99, 127	0
1	E	400/448 (89%)	-0.47	2 (0%) 87 76	25, 53, 93, 129	0
1	F	400/448 (89%)	-0.46	0 100 100	31, 60, 95, 119	0
1	G	400/448 (89%)	-0.49	0 100 100	27, 59, 92, 120	0
1	H	400/448 (89%)	-0.47	0 100 100	27, 58, 91, 125	0
2	I	0/8	-	-	-	-
3	J	0/6	-	-	-	-
3	L	0/6	-	-	-	-
4	K	0/7	-	-	-	-
4	M	0/7	-	-	-	-
4	N	0/7	-	-	-	-
4	O	0/7	-	-	-	-
4	P	0/7	-	-	-	-
5	Q	0/3	-	-	-	-
5	R	0/3	-	-	-	-
5	S	0/3	-	-	-	-
5	T	0/3	-	-	-	-
5	U	0/3	-	-	-	-
5	V	0/3	-	-	-	-
All	All	3199/3657 (87%)	-0.50	5 (0%) 91 85	22, 56, 92, 129	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	417	GLY	3.1
1	D	416	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	417	GLY	2.6
1	B	212	TYR	2.3
1	E	29	TYR	2.1

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.