



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2024 – 12:18 PM EDT

PDB ID : 8V5P
Title : Crystal Structure of the C-terminal domain of the VZV gE ectodomain in complex with the Fab of human antibody 5A2
Authors : Harshbarger, W.; Malito, E.
Deposited on : 2023-11-30
Resolution : 4.33 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

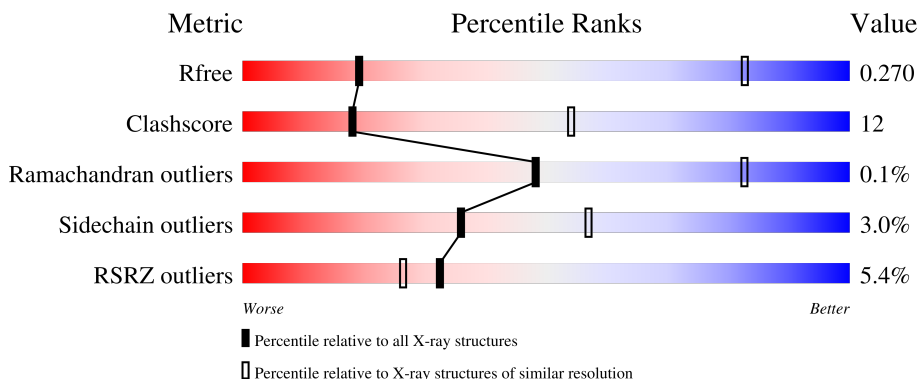
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.33 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}	164625	1019 (4.80-3.88)
Clashscore	180529	1038 (4.76-3.90)
Ramachandran outliers	177936	1011 (4.80-3.86)
Sidechain outliers	177891	1014 (4.84-3.84)
RSRZ outliers	164620	1016 (4.80-3.88)

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	254	 2% 48% 19% 31%
1	C	254	 3% 45% 22% 31%
1	D	254	 % 46% 23% 31%
1	G	254	 2% 43% 25% 31%
2	E	242	 10% 71% 17% 12%

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Mol	Chain	Length	Quality of chain
2	F	242	<p>2% 72% 16% 12%</p>
2	H	242	<p>1% 69% 18% 12%</p>
2	J	242	<p>4% 60% 28% 12%</p>
3	I	210	<p>2% 76% 22%</p>
3	L	210	<p>3% 71% 28%</p>
3	X	210	<p>9% 73% 26%</p>
3	Y	210	<p>21% 76% 23%</p>

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 18368 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 Envelope glycoprotein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	175	1396	899	230	256	11	0	0	0
1	D	175	1396	899	230	256	11	0	0	0
1	G	175	1396	899	230	256	11	0	0	0
1	C	175	1396	899	230	256	11	0	0	0

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	271	MET	-	initiating methionine	UNP A0A1B1JEP3
A	272	GLY	-	expression tag	UNP A0A1B1JEP3
A	273	THR	-	expression tag	UNP A0A1B1JEP3
A	274	VAL	-	expression tag	UNP A0A1B1JEP3
A	275	ASN	-	expression tag	UNP A0A1B1JEP3
A	276	LYS	-	expression tag	UNP A0A1B1JEP3
A	277	PRO	-	expression tag	UNP A0A1B1JEP3
A	278	VAL	-	expression tag	UNP A0A1B1JEP3
A	279	VAL	-	expression tag	UNP A0A1B1JEP3
A	280	GLY	-	expression tag	UNP A0A1B1JEP3
A	281	VAL	-	expression tag	UNP A0A1B1JEP3
A	282	LEU	-	expression tag	UNP A0A1B1JEP3
A	283	MET	-	expression tag	UNP A0A1B1JEP3
A	284	GLY	-	expression tag	UNP A0A1B1JEP3
A	285	PHE	-	expression tag	UNP A0A1B1JEP3
A	286	GLY	-	expression tag	UNP A0A1B1JEP3
A	287	ILE	-	expression tag	UNP A0A1B1JEP3
A	288	ILE	-	expression tag	UNP A0A1B1JEP3
A	289	THR	-	expression tag	UNP A0A1B1JEP3
A	290	GLY	-	expression tag	UNP A0A1B1JEP3
A	291	THR	-	expression tag	UNP A0A1B1JEP3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	292	LEU	-	expression tag	UNP A0A1B1JEP3
A	293	ARG	-	expression tag	UNP A0A1B1JEP3
A	294	ILE	-	expression tag	UNP A0A1B1JEP3
A	295	THR	-	expression tag	UNP A0A1B1JEP3
A	296	ASN	-	expression tag	UNP A0A1B1JEP3
A	297	PRO	-	expression tag	UNP A0A1B1JEP3
A	298	VAL	-	expression tag	UNP A0A1B1JEP3
A	299	ARG	-	expression tag	UNP A0A1B1JEP3
A	300	ALA	-	expression tag	UNP A0A1B1JEP3
A	517	GLY	-	expression tag	UNP A0A1B1JEP3
A	518	SER	-	expression tag	UNP A0A1B1JEP3
A	519	HIS	-	expression tag	UNP A0A1B1JEP3
A	520	HIS	-	expression tag	UNP A0A1B1JEP3
A	521	HIS	-	expression tag	UNP A0A1B1JEP3
A	522	HIS	-	expression tag	UNP A0A1B1JEP3
A	523	HIS	-	expression tag	UNP A0A1B1JEP3
A	524	HIS	-	expression tag	UNP A0A1B1JEP3
D	271	MET	-	initiating methionine	UNP A0A1B1JEP3
D	272	GLY	-	expression tag	UNP A0A1B1JEP3
D	273	THR	-	expression tag	UNP A0A1B1JEP3
D	274	VAL	-	expression tag	UNP A0A1B1JEP3
D	275	ASN	-	expression tag	UNP A0A1B1JEP3
D	276	LYS	-	expression tag	UNP A0A1B1JEP3
D	277	PRO	-	expression tag	UNP A0A1B1JEP3
D	278	VAL	-	expression tag	UNP A0A1B1JEP3
D	279	VAL	-	expression tag	UNP A0A1B1JEP3
D	280	GLY	-	expression tag	UNP A0A1B1JEP3
D	281	VAL	-	expression tag	UNP A0A1B1JEP3
D	282	LEU	-	expression tag	UNP A0A1B1JEP3
D	283	MET	-	expression tag	UNP A0A1B1JEP3
D	284	GLY	-	expression tag	UNP A0A1B1JEP3
D	285	PHE	-	expression tag	UNP A0A1B1JEP3
D	286	GLY	-	expression tag	UNP A0A1B1JEP3
D	287	ILE	-	expression tag	UNP A0A1B1JEP3
D	288	ILE	-	expression tag	UNP A0A1B1JEP3
D	289	THR	-	expression tag	UNP A0A1B1JEP3
D	290	GLY	-	expression tag	UNP A0A1B1JEP3
D	291	THR	-	expression tag	UNP A0A1B1JEP3
D	292	LEU	-	expression tag	UNP A0A1B1JEP3
D	293	ARG	-	expression tag	UNP A0A1B1JEP3
D	294	ILE	-	expression tag	UNP A0A1B1JEP3
D	295	THR	-	expression tag	UNP A0A1B1JEP3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	296	ASN	-	expression tag	UNP A0A1B1JEP3
D	297	PRO	-	expression tag	UNP A0A1B1JEP3
D	298	VAL	-	expression tag	UNP A0A1B1JEP3
D	299	ARG	-	expression tag	UNP A0A1B1JEP3
D	300	ALA	-	expression tag	UNP A0A1B1JEP3
D	517	GLY	-	expression tag	UNP A0A1B1JEP3
D	518	SER	-	expression tag	UNP A0A1B1JEP3
D	519	HIS	-	expression tag	UNP A0A1B1JEP3
D	520	HIS	-	expression tag	UNP A0A1B1JEP3
D	521	HIS	-	expression tag	UNP A0A1B1JEP3
D	522	HIS	-	expression tag	UNP A0A1B1JEP3
D	523	HIS	-	expression tag	UNP A0A1B1JEP3
D	524	HIS	-	expression tag	UNP A0A1B1JEP3
G	271	MET	-	initiating methionine	UNP A0A1B1JEP3
G	272	GLY	-	expression tag	UNP A0A1B1JEP3
G	273	THR	-	expression tag	UNP A0A1B1JEP3
G	274	VAL	-	expression tag	UNP A0A1B1JEP3
G	275	ASN	-	expression tag	UNP A0A1B1JEP3
G	276	LYS	-	expression tag	UNP A0A1B1JEP3
G	277	PRO	-	expression tag	UNP A0A1B1JEP3
G	278	VAL	-	expression tag	UNP A0A1B1JEP3
G	279	VAL	-	expression tag	UNP A0A1B1JEP3
G	280	GLY	-	expression tag	UNP A0A1B1JEP3
G	281	VAL	-	expression tag	UNP A0A1B1JEP3
G	282	LEU	-	expression tag	UNP A0A1B1JEP3
G	283	MET	-	expression tag	UNP A0A1B1JEP3
G	284	GLY	-	expression tag	UNP A0A1B1JEP3
G	285	PHE	-	expression tag	UNP A0A1B1JEP3
G	286	GLY	-	expression tag	UNP A0A1B1JEP3
G	287	ILE	-	expression tag	UNP A0A1B1JEP3
G	288	ILE	-	expression tag	UNP A0A1B1JEP3
G	289	THR	-	expression tag	UNP A0A1B1JEP3
G	290	GLY	-	expression tag	UNP A0A1B1JEP3
G	291	THR	-	expression tag	UNP A0A1B1JEP3
G	292	LEU	-	expression tag	UNP A0A1B1JEP3
G	293	ARG	-	expression tag	UNP A0A1B1JEP3
G	294	ILE	-	expression tag	UNP A0A1B1JEP3
G	295	THR	-	expression tag	UNP A0A1B1JEP3
G	296	ASN	-	expression tag	UNP A0A1B1JEP3
G	297	PRO	-	expression tag	UNP A0A1B1JEP3
G	298	VAL	-	expression tag	UNP A0A1B1JEP3
G	299	ARG	-	expression tag	UNP A0A1B1JEP3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	300	ALA	-	expression tag	UNP A0A1B1JEP3
G	517	GLY	-	expression tag	UNP A0A1B1JEP3
G	518	SER	-	expression tag	UNP A0A1B1JEP3
G	519	HIS	-	expression tag	UNP A0A1B1JEP3
G	520	HIS	-	expression tag	UNP A0A1B1JEP3
G	521	HIS	-	expression tag	UNP A0A1B1JEP3
G	522	HIS	-	expression tag	UNP A0A1B1JEP3
G	523	HIS	-	expression tag	UNP A0A1B1JEP3
G	524	HIS	-	expression tag	UNP A0A1B1JEP3
C	271	MET	-	initiating methionine	UNP A0A1B1JEP3
C	272	GLY	-	expression tag	UNP A0A1B1JEP3
C	273	THR	-	expression tag	UNP A0A1B1JEP3
C	274	VAL	-	expression tag	UNP A0A1B1JEP3
C	275	ASN	-	expression tag	UNP A0A1B1JEP3
C	276	LYS	-	expression tag	UNP A0A1B1JEP3
C	277	PRO	-	expression tag	UNP A0A1B1JEP3
C	278	VAL	-	expression tag	UNP A0A1B1JEP3
C	279	VAL	-	expression tag	UNP A0A1B1JEP3
C	280	GLY	-	expression tag	UNP A0A1B1JEP3
C	281	VAL	-	expression tag	UNP A0A1B1JEP3
C	282	LEU	-	expression tag	UNP A0A1B1JEP3
C	283	MET	-	expression tag	UNP A0A1B1JEP3
C	284	GLY	-	expression tag	UNP A0A1B1JEP3
C	285	PHE	-	expression tag	UNP A0A1B1JEP3
C	286	GLY	-	expression tag	UNP A0A1B1JEP3
C	287	ILE	-	expression tag	UNP A0A1B1JEP3
C	288	ILE	-	expression tag	UNP A0A1B1JEP3
C	289	THR	-	expression tag	UNP A0A1B1JEP3
C	290	GLY	-	expression tag	UNP A0A1B1JEP3
C	291	THR	-	expression tag	UNP A0A1B1JEP3
C	292	LEU	-	expression tag	UNP A0A1B1JEP3
C	293	ARG	-	expression tag	UNP A0A1B1JEP3
C	294	ILE	-	expression tag	UNP A0A1B1JEP3
C	295	THR	-	expression tag	UNP A0A1B1JEP3
C	296	ASN	-	expression tag	UNP A0A1B1JEP3
C	297	PRO	-	expression tag	UNP A0A1B1JEP3
C	298	VAL	-	expression tag	UNP A0A1B1JEP3
C	299	ARG	-	expression tag	UNP A0A1B1JEP3
C	300	ALA	-	expression tag	UNP A0A1B1JEP3
C	517	GLY	-	expression tag	UNP A0A1B1JEP3
C	518	SER	-	expression tag	UNP A0A1B1JEP3
C	519	HIS	-	expression tag	UNP A0A1B1JEP3

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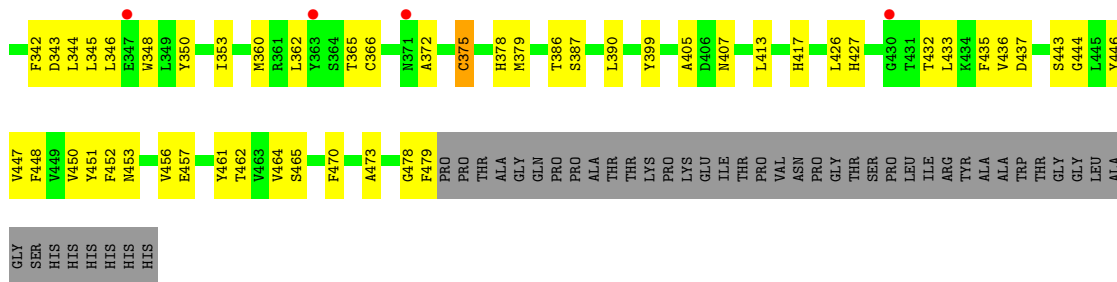
Chain	Residue	Modelled	Actual	Comment	Reference
C	520	HIS	-	expression tag	UNP A0A1B1JEP3
C	521	HIS	-	expression tag	UNP A0A1B1JEP3
C	522	HIS	-	expression tag	UNP A0A1B1JEP3
C	523	HIS	-	expression tag	UNP A0A1B1JEP3
C	524	HIS	-	expression tag	UNP A0A1B1JEP3

- Molecule 2 is a protein called 5A2 Fab heavy chain.

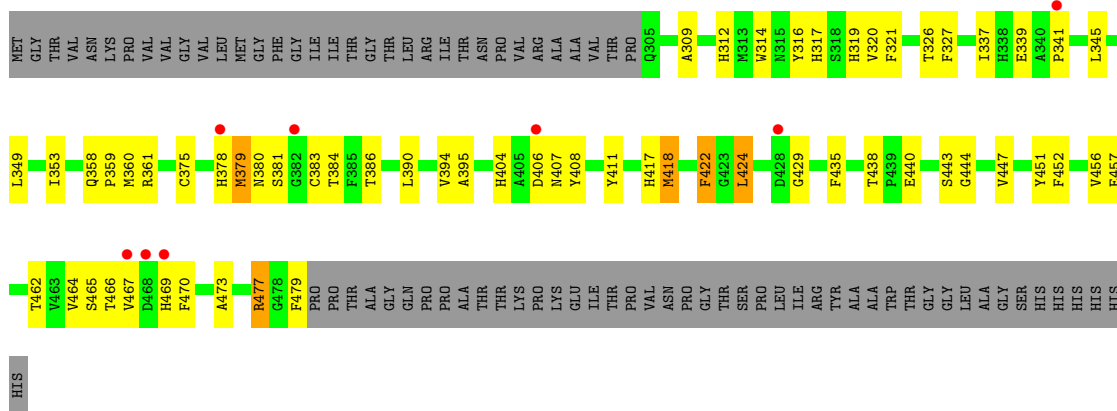
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	214	1616	1026	271	315	4	0	0	0
2	E	214	1616	1026	271	315	4	0	0	0
2	J	214	1616	1026	271	315	4	0	0	0
2	F	214	1616	1026	271	315	4	0	0	0

- Molecule 3 is a protein called 5A2 Fab Light Chain.

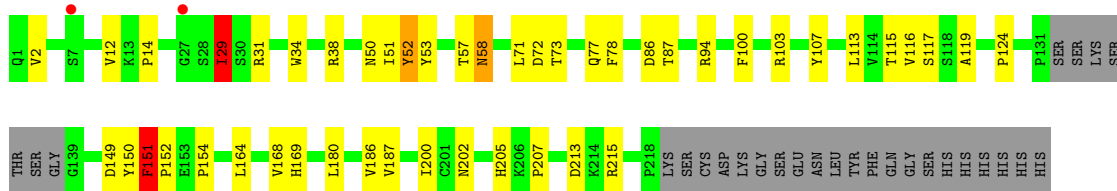
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	210	1580	995	260	320	5	0	0	0
3	Y	210	1580	995	260	320	5	0	0	0
3	X	210	1580	995	260	320	5	0	0	0
3	I	210	1580	995	260	320	5	0	0	0



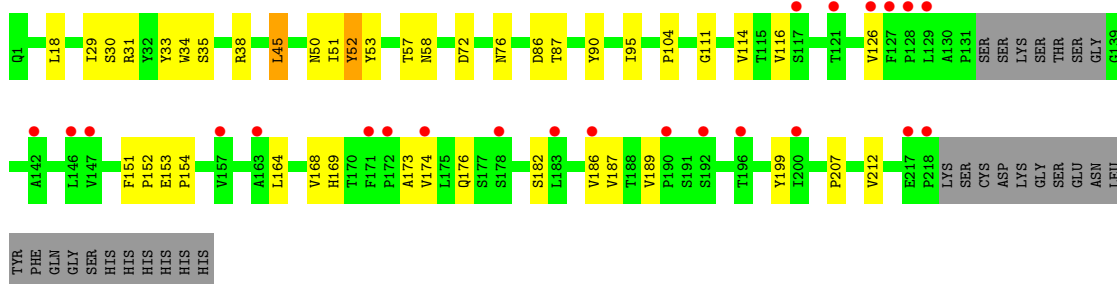
• Molecule 1: Envelope glycoprotein E



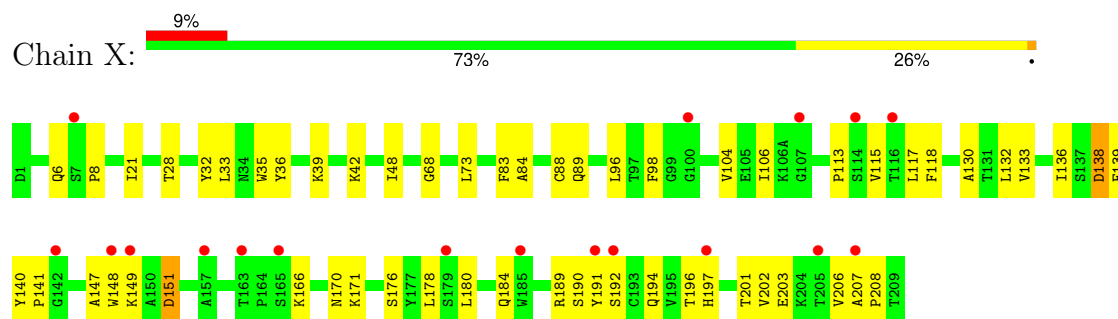
• Molecule 2: 5A2 Fab heavy chain



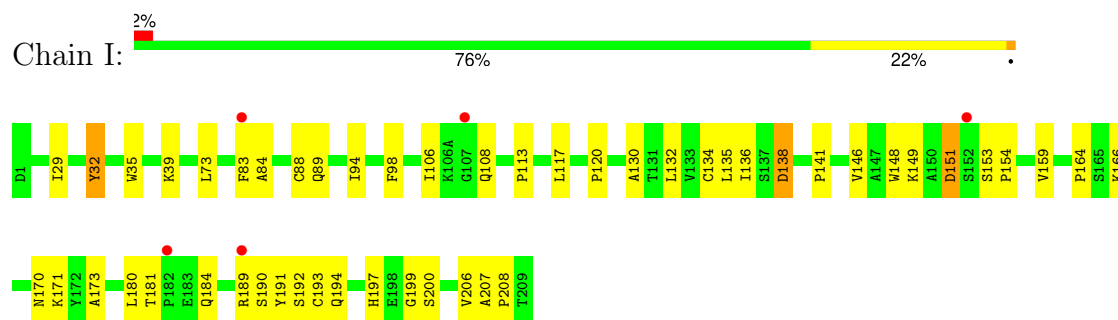
• Molecule 2: 5A2 Fab heavy chain



- Molecule 3: 5A2 Fab Light Chain



- Molecule 3: 5A2 Fab Light Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	274.82Å 274.82Å 128.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.80 – 4.33 45.80 – 4.33	Depositor EDS
% Data completeness (in resolution range)	99.0 (45.80-4.33) 97.3 (45.80-4.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.70 (at 4.29Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.222 , 0.272 0.222 , 0.270	Depositor DCC
R_{free} test set	31417 reflections (6.01%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtrriage
Anisotropy	0.004	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 106.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	18368	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% 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	0.28	0/1444	0.57	0/1974
1	C	0.28	0/1444	0.59	0/1974
1	D	0.28	0/1444	0.56	0/1974
1	G	0.28	0/1444	0.56	0/1974
2	E	0.25	0/1657	0.52	0/2268
2	F	0.26	0/1657	0.54	0/2268
2	H	0.26	0/1657	0.55	0/2268
2	J	0.27	0/1657	0.56	0/2268
3	I	0.27	0/1618	0.56	0/2208
3	L	0.27	0/1618	0.53	0/2208
3	X	0.26	0/1618	0.52	1/2208 (0.0%)
3	Y	0.26	0/1618	0.52	0/2208
All	All	0.27	0/18876	0.55	1/25800 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	F	0	1
2	H	0	2
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	X	33	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	429	GLY	Peptide
2	F	151	PHE	Peptide
2	H	151	PHE	Peptide
2	H	29	ILE	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1396	0	1297	38	0
1	C	1396	0	1297	42	0
1	D	1396	0	1297	40	0
1	G	1396	0	1297	47	0
2	E	1616	0	1594	26	0
2	F	1616	0	1594	23	0
2	H	1616	0	1594	30	0
2	J	1616	0	1594	50	0
3	I	1580	0	1553	44	0
3	L	1580	0	1553	38	0
3	X	1580	0	1553	47	0
3	Y	1580	0	1553	44	0
All	All	18368	0	17776	434	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 12.

All (434) 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)
3:I:164:PRO:HG3	3:I:173:ALA:H	1.33	0.93
1:A:397:THR:HG21	1:A:430:GLY:HA3	1.56	0.88
3:X:83:PHE:HB3	3:X:166:LYS:HD2	1.58	0.85
3:L:150:LYS:HB2	3:L:193:SER:HB3	1.58	0.84
3:L:133:LEU:HD11	3:L:149:TRP:HE1	1.42	0.83
3:Y:106:ILE:O	3:Y:140:TYR:OH	1.99	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:83:PHE:O	3:I:166:LYS:NZ	2.14	0.80
1:C:440:GLU:HG3	1:C:467:VAL:HG11	1.64	0.79
3:X:139:PHE:HD2	3:X:141:PRO:HD2	1.48	0.79
2:H:72:ASP:HB3	2:H:77:GLN:HG3	1.65	0.79
2:J:23:ILE:HA	2:J:77:GLN:NE2	1.98	0.78
2:H:113:LEU:HD23	2:H:154:PRO:HD3	1.66	0.78
3:L:167:LYS:HG2	3:L:173:TYR:HE1	1.49	0.77
1:A:362:LEU:HD11	1:A:473:ALA:HB1	1.68	0.75
3:I:149:LYS:HB2	3:I:192:SER:HB2	1.68	0.75
3:Y:139:PHE:HD2	3:Y:141:PRO:HD2	1.52	0.74
2:F:164:LEU:HD21	2:F:187:VAL:HG11	1.70	0.74
3:Y:141:PRO:HG2	3:Y:197:HIS:HD2	1.52	0.74
2:H:119:ALA:HB3	2:H:151:PHE:HE2	1.53	0.73
3:Y:132:LEU:HD11	3:Y:148:TRP:HE1	1.54	0.73
3:L:21:ILE:HD11	3:L:73:LEU:HD23	1.72	0.72
1:G:309:ALA:HB1	1:G:337:ILE:HG22	1.72	0.72
1:D:435:PHE:HB3	1:D:438:THR:HG21	1.70	0.71
1:C:407:ASN:ND2	1:C:411:TYR:OH	2.22	0.71
1:A:345:LEU:HB3	1:A:451:TYR:HB2	1.72	0.71
3:X:106:ILE:O	3:X:140:TYR:OH	2.04	0.70
3:Y:106:ILE:HD11	3:Y:166:LYS:HG3	1.74	0.70
1:A:392:GLN:NE2	1:C:418:MET:SD	2.65	0.69
1:D:348:TRP:HB2	1:D:395:ALA:HB3	1.74	0.69
1:A:386:THR:HG22	1:A:387:SER:H	1.58	0.69
1:D:397:THR:HG21	1:D:430:GLY:HA3	1.74	0.69
3:Y:29:ILE:HG23	3:Y:92:TYR:HB2	1.74	0.69
3:L:39:LYS:HG3	3:L:84:ALA:HB2	1.74	0.68
3:Y:149:LYS:HB2	3:Y:192:SER:HB2	1.75	0.68
3:L:165:PRO:HD3	3:L:174:ALA:O	1.94	0.68
1:C:312:HIS:NE2	3:I:32:TYR:OH	2.26	0.68
3:X:149:LYS:HB2	3:X:192:SER:HB2	1.76	0.68
2:F:113:LEU:HD23	2:F:154:PRO:HD3	1.76	0.68
3:L:2:ILE:O	3:L:97:THR:HG21	1.93	0.67
1:G:372:ALA:HB3	1:G:375:CYS:HB2	1.76	0.67
1:D:345:LEU:HB3	1:D:451:TYR:HB2	1.76	0.66
1:A:389:HIS:CG	1:D:415:ILE:HD11	2.30	0.66
1:G:319:HIS:HB3	1:G:464:VAL:HG23	1.77	0.66
3:X:184:GLN:O	3:X:191:TYR:OH	2.13	0.66
2:H:164:LEU:HD21	2:H:187:VAL:HG11	1.78	0.66
3:X:106:ILE:HD11	3:X:166:LYS:HG3	1.76	0.66
3:Y:21:ILE:HD11	3:Y:73:LEU:HD23	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:422:PHE:HB2	1:C:424:LEU:HD22	1.79	0.65
3:X:106:ILE:HD13	3:X:170:ASN:HA	1.77	0.65
1:C:358:GLN:HB2	1:C:359:PRO:HD3	1.78	0.65
3:Y:83:PHE:HB3	3:Y:166:LYS:HD2	1.77	0.65
1:C:435:PHE:HB3	1:C:438:THR:HG21	1.78	0.64
2:F:200:ILE:HG12	2:F:215:ARG:HG3	1.78	0.64
1:G:345:LEU:HB3	1:G:451:TYR:HB2	1.80	0.64
1:G:350:TYR:HE1	1:G:444:GLY:HA3	1.63	0.64
3:I:148:TRP:HD1	3:I:159:VAL:HG12	1.62	0.64
1:A:439:PRO:HD2	1:A:442:LEU:HD12	1.79	0.64
1:D:360:MET:HB3	1:D:473:ALA:HA	1.78	0.64
1:C:349:LEU:HB2	1:C:447:VAL:HG22	1.80	0.63
1:D:420:PRO:HG3	1:C:417:HIS:NE2	2.13	0.63
1:C:394:VAL:HG22	1:C:395:ALA:H	1.64	0.63
1:C:353:ILE:HG22	1:C:444:GLY:HA2	1.81	0.62
3:Y:115:VAL:O	3:Y:204:LYS:NZ	2.32	0.62
2:H:200:ILE:HG12	2:H:215:ARG:HG3	1.81	0.62
3:I:141:PRO:HB2	3:I:197:HIS:HE1	1.63	0.62
1:A:311:PHE:HD2	1:A:333:LEU:HD11	1.65	0.62
1:A:348:TRP:HB2	1:A:395:ALA:HB3	1.82	0.62
3:L:80:PRO:HA	3:L:106:ILE:HD13	1.82	0.62
3:Y:151:ASP:OD2	3:Y:190:SER:N	2.32	0.61
3:Y:141:PRO:HG2	3:Y:197:HIS:CD2	2.33	0.61
1:D:395:ALA:HB1	1:D:426:LEU:HD21	1.82	0.61
1:G:386:THR:OG1	1:G:387:SER:N	2.32	0.61
3:I:181:THR:OG1	3:I:184:GLN:OE1	2.19	0.60
1:A:313:MET:HG3	1:A:333:LEU:HD13	1.82	0.60
2:J:84:ALA:HA	2:J:116:VAL:HG21	1.83	0.60
3:L:149:TRP:CD1	3:L:179:LEU:HD22	2.36	0.60
3:X:113:PRO:HB3	3:X:139:PHE:HB3	1.83	0.60
1:G:337:ILE:HD11	1:G:405:ALA:O	2.00	0.60
2:J:200:ILE:HG12	2:J:215:ARG:HG3	1.84	0.60
1:C:345:LEU:HB3	1:C:451:TYR:HB2	1.84	0.60
3:L:109:GLN:HG3	3:L:171:ASN:HB2	1.83	0.59
3:Y:113:PRO:HB3	3:Y:139:PHE:HB3	1.84	0.59
1:C:321:PHE:N	1:C:466:THR:HG23	2.17	0.59
3:I:134:CYS:HB2	3:I:148:TRP:CH2	2.37	0.59
3:X:196:THR:HG22	3:X:201:THR:HA	1.84	0.59
3:X:21:ILE:HD11	3:X:73:LEU:HD23	1.84	0.59
1:C:404:HIS:ND1	1:C:411:TYR:OH	2.36	0.58
3:L:15:VAL:HG23	3:L:108:GLY:HA3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:164:LEU:HD21	2:J:187:VAL:HG11	1.85	0.58
1:C:353:ILE:HG23	1:C:469:HIS:HE2	1.69	0.58
3:L:36:TYR:HE2	3:L:89:GLN:HB3	1.69	0.57
1:G:348:TRP:CD2	1:G:433:LEU:HD11	2.39	0.57
2:J:152:PRO:HB2	2:J:205:HIS:HE2	1.68	0.57
1:G:312:HIS:CG	3:X:32:TYR:HH	2.21	0.56
1:G:399:TYR:HE1	1:G:413:LEU:HD12	1.70	0.56
1:G:362:LEU:HD13	1:G:461:TYR:CD2	2.40	0.56
2:J:99:SER:HB3	2:J:102:GLU:HG3	1.87	0.56
1:C:375:CYS:O	1:C:386:THR:OG1	2.20	0.56
2:H:2:VAL:HG22	2:H:107:TYR:HD2	1.69	0.56
2:J:194:LEU:HD21	2:J:218:PRO:HG2	1.88	0.56
3:X:139:PHE:CD2	3:X:141:PRO:HD2	2.36	0.56
1:A:314:TRP:HZ3	2:H:50:ASN:HD21	1.54	0.56
1:A:346:LEU:HB2	1:A:397:THR:OG1	2.06	0.56
3:I:89:GLN:HB2	3:I:98:PHE:CD2	2.41	0.56
1:G:346:LEU:HD22	1:G:450:VAL:HG12	1.86	0.56
3:I:120:PRO:HD3	3:I:132:LEU:HB3	1.88	0.56
3:L:89:GLN:HB2	3:L:98:PHE:CD2	2.41	0.55
2:J:106:ASP:OD1	2:J:106:ASP:N	2.40	0.55
3:I:151:ASP:OD2	3:I:190:SER:N	2.36	0.55
1:A:316:TYR:HB2	3:L:94:ILE:HB	1.88	0.55
2:J:149:ASP:HA	2:J:180:LEU:HB3	1.88	0.55
2:J:38:ARG:NH1	2:J:86:ASP:OD1	2.40	0.55
3:I:148:TRP:CD1	3:I:159:VAL:HG12	2.42	0.55
1:G:326:THR:HG23	1:G:436:VAL:HG12	1.89	0.55
1:G:312:HIS:CE1	3:X:32:TYR:HH	2.19	0.55
1:G:447:VAL:HG12	1:G:461:TYR:HD1	1.72	0.55
1:C:320:VAL:HB	1:C:466:THR:HG22	1.89	0.54
1:A:334:GLN:HG3	2:H:103:ARG:NH2	2.22	0.54
3:X:138:ASP:HA	3:X:171:LYS:HB3	1.90	0.54
1:A:334:GLN:HG3	2:H:103:ARG:HH22	1.73	0.54
2:H:205:HIS:CD2	2:H:207:PRO:HD2	2.43	0.54
3:I:39:LYS:HG3	3:I:84:ALA:HB2	1.90	0.54
1:D:343:ASP:OD1	1:D:343:ASP:N	2.38	0.54
1:C:309:ALA:HB1	1:C:337:ILE:HG22	1.90	0.54
1:C:465:SER:OG	1:C:469:HIS:HB3	2.06	0.54
2:F:153:GLU:HG3	2:F:181:TYR:CE2	2.42	0.54
2:E:126:VAL:HG21	2:E:212:VAL:HG11	1.90	0.53
1:G:327:PHE:CZ	1:G:435:PHE:HE1	2.26	0.53
1:G:365:THR:O	1:G:365:THR:OG1	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:447:VAL:HG12	1:G:461:TYR:CD1	2.43	0.53
3:I:138:ASP:HA	3:I:171:LYS:HB3	1.88	0.53
1:D:465:SER:HB2	1:D:469:HIS:HB2	1.89	0.53
2:E:38:ARG:NH1	2:E:86:ASP:OD1	2.41	0.53
2:H:38:ARG:NH1	2:H:86:ASP:OD1	2.42	0.53
1:D:427:HIS:NE2	1:D:434:LYS:HD2	2.23	0.53
2:E:169:HIS:HB2	2:E:186:VAL:HG12	1.89	0.53
1:G:329:LEU:HD21	1:G:462:THR:HG21	1.89	0.53
3:I:184:GLN:O	3:I:191:TYR:OH	2.26	0.53
1:D:367:LEU:HG	1:D:388:PRO:HD3	1.89	0.53
2:J:35:SER:HB2	2:J:50:ASN:HB3	1.89	0.53
2:J:168:VAL:HG22	2:J:187:VAL:HG22	1.89	0.53
2:F:168:VAL:HG22	2:F:187:VAL:HG22	1.91	0.53
3:I:108:GLN:HG3	3:I:170:ASN:HB2	1.91	0.53
2:E:30:SER:O	2:E:31:ARG:HG2	2.09	0.52
1:A:316:TYR:O	2:H:58:ASN:ND2	2.42	0.52
1:A:397:THR:HG22	1:A:416:SER:HB2	1.89	0.52
1:D:319:HIS:HB3	1:D:464:VAL:HG22	1.91	0.52
1:G:320:VAL:HA	1:G:465:SER:O	2.09	0.52
1:D:466:THR:OG1	1:D:467:VAL:N	2.43	0.52
1:G:446:TYR:HB2	1:G:462:THR:HG23	1.92	0.52
3:L:106:ILE:HB	3:L:167:LYS:HE2	1.91	0.51
2:E:154:PRO:HG2	2:E:207:PRO:HG2	1.92	0.51
2:J:77:GLN:NE2	2:J:77:GLN:HA	2.25	0.51
2:F:33:TYR:HB2	2:F:95:ILE:HB	1.92	0.51
3:I:141:PRO:HB2	3:I:197:HIS:CE1	2.44	0.51
2:J:129:LEU:HD22	3:X:118:PHE:HB3	1.93	0.51
3:X:140:TYR:CG	3:X:140:TYR:O	2.64	0.51
1:D:314:TRP:O	1:D:317:HIS:NE2	2.44	0.51
3:X:151:ASP:OD2	3:X:190:SER:N	2.42	0.51
1:C:360:MET:HB3	1:C:473:ALA:HA	1.91	0.51
2:F:205:HIS:CD2	2:F:207:PRO:HD2	2.45	0.51
2:J:22:CYS:O	2:J:77:GLN:HG3	2.09	0.51
3:X:84:ALA:O	3:X:104:VAL:HG12	2.11	0.51
2:J:45:LEU:HD23	2:J:45:LEU:H	1.76	0.51
1:D:314:TRP:CZ3	3:Y:94:ILE:HD11	2.46	0.50
3:X:113:PRO:HG3	3:X:197:HIS:HE1	1.77	0.50
1:C:477:ARG:H	1:C:477:ARG:HD3	1.75	0.50
2:H:51:ILE:HG12	2:H:52:TYR:O	2.11	0.50
2:E:189:VAL:HG11	2:E:199:TYR:CE1	2.47	0.50
2:J:150:TYR:O	2:J:181:TYR:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:113:PRO:HG3	3:X:197:HIS:CE1	2.46	0.50
1:C:317:HIS:HB2	1:C:462:THR:HB	1.92	0.50
1:D:335:TYR:OH	1:D:408:TYR:HA	2.12	0.50
3:X:190:SER:HA	3:X:206:VAL:O	2.12	0.50
3:X:141:PRO:HG2	3:X:197:HIS:CD2	2.46	0.50
3:Y:148:TRP:CD1	3:Y:178:LEU:HD22	2.47	0.50
3:Y:184:GLN:O	3:Y:191:TYR:OH	2.30	0.49
1:G:452:PHE:HB3	1:G:457:GLU:HG3	1.94	0.49
3:X:189:ARG:O	3:X:207:ALA:HA	2.12	0.49
2:F:99:SER:HB3	2:F:102:GLU:HG3	1.94	0.49
1:D:329:LEU:HD21	1:D:462:THR:HG21	1.95	0.49
3:Y:106:ILE:HD13	3:Y:170:ASN:HA	1.93	0.49
1:D:427:HIS:HB2	1:D:432:THR:HG23	1.93	0.49
2:J:90:TYR:O	2:J:111:GLY:HA2	2.12	0.49
3:I:148:TRP:CZ3	3:I:193:CYS:HB2	2.48	0.49
1:G:334:GLN:OE1	2:J:103:ARG:NE	2.45	0.49
3:I:189:ARG:O	3:I:208:PRO:HD3	2.13	0.49
1:D:420:PRO:HG3	1:C:417:HIS:CD2	2.47	0.49
2:J:6:GLU:N	2:J:6:GLU:OE1	2.45	0.49
1:A:397:THR:HG22	1:A:416:SER:CB	2.42	0.49
2:J:72:ASP:O	2:J:76:ASN:N	2.46	0.49
3:I:189:ARG:O	3:I:207:ALA:HA	2.12	0.49
2:H:2:VAL:HG22	2:H:107:TYR:CD2	2.47	0.48
2:E:51:ILE:HG13	2:E:57:THR:HG22	1.95	0.48
1:C:326:THR:HA	1:C:435:PHE:O	2.13	0.48
2:F:151:PHE:HB3	2:F:152:PRO:HD3	1.95	0.48
2:F:149:ASP:HA	2:F:180:LEU:HB3	1.95	0.48
2:J:24:VAL:H	2:J:77:GLN:NE2	2.10	0.48
2:E:45:LEU:HD23	2:E:45:LEU:H	1.78	0.48
3:Y:35:TRP:O	3:Y:47:LEU:HG	2.14	0.48
3:Y:36:TYR:HE2	3:Y:89:GLN:HB3	1.78	0.48
3:Y:148:TRP:HD1	3:Y:178:LEU:HD22	1.79	0.48
3:X:130:ALA:HB3	3:X:180:LEU:O	2.14	0.48
1:C:321:PHE:H	1:C:466:THR:HG23	1.79	0.48
1:D:326:THR:HG23	1:D:436:VAL:HG12	1.95	0.48
3:Y:139:PHE:CD2	3:Y:141:PRO:HD2	2.41	0.48
1:A:424:LEU:HD11	1:A:435:PHE:CE2	2.49	0.48
2:H:71:LEU:HD12	2:H:78:PHE:HB3	1.96	0.48
3:Y:47:LEU:HD12	3:Y:48:ILE:HG12	1.95	0.48
2:J:169:HIS:HB2	2:J:186:VAL:HG12	1.94	0.48
2:J:177:SER:C	2:J:179:GLY:H	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:HIS:HB2	1:A:462:THR:HB	1.95	0.48
2:H:100:PHE:O	3:L:32:TYR:OH	2.32	0.48
1:G:314:TRP:HH2	3:X:96:LEU:HD21	1.78	0.48
1:G:353:ILE:HG12	1:G:444:GLY:HA2	1.96	0.48
3:X:147:ALA:HB3	3:X:194:GLN:HB3	1.95	0.47
3:L:8:PRO:HD2	3:L:21:ILE:HG22	1.96	0.47
1:D:447:VAL:HG12	1:D:461:TYR:HD1	1.79	0.47
1:C:314:TRP:CD2	3:I:94:ILE:HD11	2.48	0.47
1:G:309:ALA:C	1:G:310:GLU:OE1	2.53	0.47
1:G:312:HIS:HE1	1:G:334:GLN:OE1	1.97	0.47
2:J:37:ILE:HD11	2:J:105:ILE:HD13	1.95	0.47
3:I:106:ILE:HD13	3:I:170:ASN:HA	1.96	0.47
1:A:318:SER:O	2:H:57:THR:N	2.46	0.47
2:H:202:ASN:ND2	2:H:213:ASP:OD1	2.47	0.47
1:G:332:HIS:CG	2:J:103:ARG:HH22	2.32	0.47
2:J:152:PRO:HD2	2:J:205:HIS:CE1	2.50	0.47
3:L:190:ARG:O	3:L:209:PRO:HD3	2.15	0.47
1:D:452:PHE:HB3	1:D:457:GLU:HG3	1.96	0.47
2:J:32:TYR:OH	2:J:94:ARG:NH1	2.47	0.47
2:F:101:GLY:HA2	3:I:32:TYR:CE2	2.49	0.47
3:I:148:TRP:O	3:I:154:PRO:HA	2.14	0.47
3:Y:136:ILE:HD11	3:Y:144:VAL:HG21	1.96	0.47
2:E:90:TYR:O	2:E:111:GLY:HA2	2.14	0.47
3:Y:19:VAL:O	3:Y:74:THR:HA	2.15	0.47
3:X:132:LEU:HD11	3:X:148:TRP:HE1	1.80	0.47
2:F:87:THR:OG1	2:F:116:VAL:HG22	2.14	0.47
3:I:146:VAL:HA	3:I:194:GLN:O	2.15	0.47
1:C:395:ALA:HA	1:C:418:MET:HA	1.96	0.47
3:Y:89:GLN:HB2	3:Y:98:PHE:CD2	2.50	0.46
1:C:435:PHE:HB3	1:C:438:THR:CG2	2.45	0.46
3:L:133:LEU:HG	3:L:179:LEU:HB3	1.97	0.46
2:E:176:GLN:NE2	2:E:182:SER:OG	2.33	0.46
1:G:427:HIS:HB3	1:G:432:THR:HG23	1.97	0.46
3:I:180:LEU:HD12	3:I:184:GLN:HB3	1.97	0.46
2:F:101:GLY:HA2	3:I:32:TYR:CZ	2.50	0.46
2:H:50:ASN:OD1	2:H:58:ASN:HB2	2.15	0.46
3:L:149:TRP:HH2	3:L:177:SER:HB3	1.80	0.46
3:X:117:LEU:HD23	3:X:206:VAL:HG13	1.97	0.46
3:X:148:TRP:CD1	3:X:178:LEU:HD22	2.50	0.46
1:A:348:TRP:CE2	1:A:433:LEU:HD13	2.50	0.46
2:H:29:ILE:HG21	2:H:73:THR:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:174:VAL:HG12	2:E:182:SER:HB2	1.98	0.46
3:X:117:LEU:HD12	3:X:133:VAL:O	2.15	0.46
2:H:12:VAL:O	2:H:116:VAL:HA	2.16	0.46
1:G:343:ASP:OD1	1:G:343:ASP:N	2.45	0.46
2:F:14:PRO:HD3	2:F:117:SER:O	2.16	0.46
2:J:154:PRO:HG2	2:J:207:PRO:HG3	1.97	0.46
3:I:113:PRO:HD3	3:I:197:HIS:HD2	1.81	0.46
2:J:5:GLN:HG3	2:J:23:ILE:HB	1.97	0.46
1:A:342:PHE:HE2	1:A:344:LEU:HG	1.80	0.46
1:D:435:PHE:HB3	1:D:438:THR:CG2	2.41	0.46
1:G:343:ASP:OD1	1:G:453:ASN:HA	2.16	0.46
1:A:325:ASP:O	1:A:438:THR:HG23	2.16	0.46
2:E:35:SER:HB2	2:E:50:ASN:HB3	1.98	0.46
1:G:386:THR:HG21	1:G:390:LEU:HD22	1.97	0.46
1:G:443:SER:HB2	1:C:378:HIS:CD2	2.51	0.46
3:X:194:GLN:NE2	3:X:203:GLU:HB3	2.31	0.46
1:C:353:ILE:HG23	1:C:469:HIS:NE2	2.30	0.46
1:C:361:ARG:HB2	1:C:384:THR:HG22	1.98	0.45
3:L:145:VAL:HG12	3:L:198:HIS:CD2	2.52	0.45
1:G:451:TYR:CE1	1:G:456:VAL:HG22	2.51	0.45
3:Y:2:ILE:HD13	3:Y:29:ILE:HD11	1.98	0.45
3:X:140:TYR:N	3:X:141:PRO:HD3	2.31	0.45
1:D:367:LEU:HB3	1:D:456:VAL:HG21	1.98	0.45
3:Y:132:LEU:HD11	3:Y:148:TRP:NE1	2.25	0.45
2:F:169:HIS:HB2	2:F:186:VAL:HG12	1.99	0.45
1:A:422:PHE:HB3	1:A:424:LEU:HD23	1.99	0.45
3:L:149:TRP:O	3:L:155:PRO:HA	2.17	0.45
3:Y:146:VAL:HB	3:Y:148:TRP:HZ3	1.81	0.45
1:A:349:LEU:HB2	1:A:447:VAL:CG2	2.46	0.45
2:E:151:PHE:HB3	2:E:152:PRO:HD3	1.98	0.45
3:X:132:LEU:HG	3:X:178:LEU:HB3	1.98	0.45
2:H:87:THR:HG23	2:H:115:THR:HG22	1.99	0.45
1:G:379:MET:HB3	1:C:469:HIS:HE1	1.82	0.45
1:A:427:HIS:HB3	1:A:432:THR:HG23	1.98	0.45
2:H:34:TRP:CZ3	2:H:94:ARG:HB2	2.52	0.45
1:D:317:HIS:O	1:D:462:THR:HA	2.17	0.45
3:X:89:GLN:HB2	3:X:98:PHE:CD2	2.51	0.45
3:L:161:GLU:O	3:L:177:SER:HA	2.17	0.45
3:Y:94:ILE:HD13	3:Y:94:ILE:HA	1.85	0.45
3:Y:113:PRO:HG3	3:Y:197:HIS:CE1	2.52	0.45
3:I:130:ALA:HB3	3:I:180:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:72:ASP:O	2:E:76:ASN:N	2.50	0.44
2:H:14:PRO:HD3	2:H:117:SER:O	2.18	0.44
3:Y:39:LYS:HD2	3:Y:42:LYS:HD3	1.99	0.44
2:J:139:GLY:O	2:J:191:SER:OG	2.34	0.44
3:X:96:LEU:HD12	3:X:96:LEU:H	1.83	0.44
1:D:446:TYR:HB2	1:D:462:THR:HG23	1.98	0.44
1:C:390:LEU:HD23	1:C:390:LEU:HA	1.82	0.44
1:C:327:PHE:CZ	1:C:464:VAL:HG21	2.52	0.44
1:A:344:LEU:HD23	1:A:344:LEU:HA	1.87	0.44
1:A:415:ILE:HD13	1:D:389:HIS:HB3	2.00	0.44
1:G:306:PRO:HB2	1:G:338:HIS:CE1	2.53	0.44
2:F:126:VAL:HG11	2:F:203:VAL:HG11	1.99	0.44
3:I:113:PRO:HB2	3:I:136:ILE:HG23	2.00	0.44
3:I:149:LYS:HA	3:I:153:SER:O	2.18	0.44
3:I:83:PHE:CE1	3:I:106:ILE:HA	2.53	0.44
2:H:149:ASP:HA	2:H:180:LEU:HB3	2.00	0.44
3:Y:11:LEU:HD11	3:Y:104:VAL:HG22	1.99	0.44
2:J:87:THR:OG1	2:J:116:VAL:HG22	2.18	0.44
2:E:168:VAL:HG22	2:E:187:VAL:HG22	2.00	0.43
2:E:173:ALA:HA	2:E:182:SER:O	2.17	0.43
1:C:451:TYR:CE1	1:C:456:VAL:HG22	2.53	0.43
1:A:367:LEU:HG	1:A:388:PRO:HD3	2.00	0.43
3:L:33:LEU:HD21	3:L:71:PHE:CG	2.53	0.43
1:D:312:HIS:CE1	1:D:314:TRP:CD1	3.06	0.43
1:D:379:MET:HE3	1:D:381:SER:O	2.17	0.43
2:E:87:THR:OG1	2:E:116:VAL:HG12	2.19	0.43
3:Y:2:ILE:HG21	3:Y:29:ILE:HD11	1.99	0.43
3:X:115:VAL:HG22	3:X:136:ILE:HG22	2.00	0.43
3:L:182:THR:OG1	3:L:185:GLN:OE1	2.34	0.43
3:X:189:ARG:O	3:X:208:PRO:HD3	2.17	0.43
3:Y:140:TYR:N	3:Y:141:PRO:HD3	2.33	0.43
3:Y:148:TRP:O	3:Y:154:PRO:HA	2.18	0.43
2:F:2:VAL:HG21	2:F:94:ARG:NH1	2.33	0.43
2:H:169:HIS:HB2	2:H:186:VAL:HG12	1.99	0.43
1:G:314:TRP:NE1	2:J:103:ARG:HD3	2.34	0.43
3:Y:106:ILE:HG21	3:Y:170:ASN:HB3	2.00	0.43
3:Y:140:TYR:O	3:Y:140:TYR:CG	2.71	0.43
2:J:126:VAL:HG21	2:J:212:VAL:HG11	2.00	0.43
1:A:337:ILE:HD12	1:A:405:ALA:HB1	2.01	0.43
3:L:116:VAL:HG22	3:L:137:ILE:HG22	1.99	0.43
3:X:28:THR:HG23	3:X:68:GLY:HA2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:39:LYS:HZ2	3:X:42:LYS:HZ3	1.66	0.43
1:C:309:ALA:CB	1:C:337:ILE:HG22	2.48	0.43
1:C:339:GLU:HB2	1:C:341:PRO:HD2	2.01	0.43
3:I:83:PHE:CG	3:I:106:ILE:HG12	2.53	0.43
3:L:23:CYS:HB2	3:L:35:TRP:CH2	2.54	0.43
3:L:28:THR:HG23	3:L:68:GLY:HA2	2.00	0.43
1:D:355:PRO:HD2	1:G:436:VAL:HG11	2.01	0.43
2:J:122:LYS:HA	2:J:122:LYS:HD2	1.83	0.43
2:F:100:PHE:O	3:I:32:TYR:OH	2.23	0.43
3:L:181:LEU:HD12	3:L:185:GLN:HB3	2.00	0.43
1:D:381:SER:HB2	1:G:426:LEU:O	2.19	0.43
1:C:379:MET:SD	1:C:380:ASN:N	2.74	0.43
1:A:349:LEU:HB2	1:A:447:VAL:HG22	2.01	0.42
2:E:153:GLU:N	2:E:154:PRO:HD2	2.34	0.42
3:X:194:GLN:NE2	3:X:202:VAL:O	2.45	0.42
1:A:376:LEU:H	1:A:376:LEU:HD23	1.85	0.42
2:E:18:LEU:HD22	2:E:114:VAL:HG11	2.01	0.42
1:C:443:SER:HB2	1:C:465:SER:HB3	2.01	0.42
1:G:317:HIS:HB2	1:G:462:THR:HB	2.02	0.42
2:J:151:PHE:HB3	2:J:152:PRO:HD3	2.00	0.42
3:L:114:PRO:HD3	3:L:198:HIS:ND1	2.35	0.42
2:J:24:VAL:H	2:J:77:GLN:HE22	1.66	0.42
3:I:35:TRP:NE1	3:I:88:CYS:HB3	2.35	0.42
1:G:344:LEU:HD23	1:G:344:LEU:HA	1.90	0.42
1:A:306:PRO:HB2	1:A:338:HIS:CD2	2.55	0.42
1:D:364:SER:HA	1:D:461:TYR:OH	2.20	0.42
2:F:51:ILE:HG12	2:F:52:TYR:O	2.19	0.42
2:E:52:TYR:HD1	2:E:53:TYR:H	1.68	0.42
3:X:35:TRP:CE2	3:X:73:LEU:HB2	2.55	0.42
3:I:136:ILE:O	3:I:173:ALA:HA	2.20	0.42
1:A:313:MET:HG2	1:A:333:LEU:HA	2.01	0.42
2:H:124:PRO:HA	2:H:150:TYR:HB3	2.02	0.42
3:X:8:PRO:HD2	3:X:21:ILE:HG22	2.01	0.42
1:A:329:LEU:HD21	1:A:462:THR:HG21	2.02	0.41
3:L:38:GLN:O	3:L:84:ALA:HB1	2.20	0.41
2:E:33:TYR:HB2	2:E:95:ILE:HB	2.02	0.41
3:Y:35:TRP:CZ3	3:Y:88:CYS:HB3	2.55	0.41
3:X:36:TYR:HE2	3:X:89:GLN:HB3	1.85	0.41
3:I:117:LEU:HD23	3:I:206:VAL:HG13	2.02	0.41
2:H:151:PHE:HB3	2:H:152:PRO:HD3	2.02	0.41
1:G:348:TRP:CZ3	1:G:448:PHE:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:PHE:HB3	1:C:457:GLU:HG3	2.01	0.41
1:A:342:PHE:CE2	1:A:344:LEU:HG	2.56	0.41
1:D:362:LEU:O	1:D:362:LEU:HD12	2.20	0.41
2:E:104:PRO:HB3	3:Y:49:TYR:HB2	2.01	0.41
2:F:30:SER:O	2:F:31:ARG:HG2	2.21	0.41
2:F:72:ASP:HB3	2:F:77:GLN:HB2	2.03	0.41
2:E:87:THR:HA	2:E:114:VAL:O	2.21	0.41
1:G:365:THR:HG21	1:G:478:GLY:H	1.86	0.41
2:J:29:ILE:HG13	2:J:34:TRP:CE2	2.56	0.41
2:J:32:TYR:HB2	2:J:95:ILE:O	2.21	0.41
3:X:6:GLN:HB2	3:X:88:CYS:SG	2.60	0.41
3:L:136:LEU:HD21	3:L:138:SER:HB2	2.03	0.41
2:E:164:LEU:HD21	2:E:187:VAL:HG11	2.02	0.41
3:Y:164:PRO:HB3	3:Y:173:ALA:O	2.20	0.41
1:G:312:HIS:CE1	2:J:103:ARG:HE	2.37	0.41
1:G:319:HIS:CD2	2:J:56:THR:H	2.38	0.41
2:J:173:ALA:HB2	2:J:183:LEU:HD12	2.03	0.41
3:I:35:TRP:CD2	3:I:73:LEU:HB2	2.56	0.41
3:X:83:PHE:CE1	3:X:106:ILE:HA	2.56	0.41
1:C:319:HIS:O	1:C:464:VAL:HA	2.21	0.41
2:F:12:VAL:O	2:F:116:VAL:HA	2.20	0.41
3:L:142:PRO:HD2	3:L:198:HIS:CE1	2.55	0.41
3:I:106:ILE:HD11	3:I:166:LYS:HB2	2.02	0.41
3:I:199:GLY:O	3:I:200:SER:OG	2.35	0.41
1:D:312:HIS:CE1	1:D:314:TRP:HD1	2.39	0.41
3:Y:21:ILE:HG13	3:Y:73:LEU:HB3	2.03	0.41
3:Y:180:LEU:HD12	3:Y:184:GLN:HB2	2.03	0.41
2:J:87:THR:HA	2:J:114:VAL:O	2.20	0.41
2:J:94:ARG:HD3	2:J:107:TYR:HB2	2.03	0.41
3:I:29:ILE:HG13	3:I:29:ILE:O	2.21	0.41
2:H:168:VAL:HG22	2:H:187:VAL:HG22	2.01	0.41
1:D:346:LEU:HD22	1:D:450:VAL:HG22	2.02	0.41
2:E:50:ASN:OD1	2:E:58:ASN:HB2	2.20	0.41
1:G:312:HIS:HE1	2:J:103:ARG:HE	1.69	0.41
3:I:35:TRP:CG	3:I:73:LEU:HD22	2.56	0.41
3:I:83:PHE:CD2	3:I:106:ILE:HG12	2.55	0.41
1:D:353:ILE:HG23	1:D:444:GLY:HA2	2.02	0.40
1:D:399:TYR:HE1	1:D:414:GLY:H	1.68	0.40
1:D:451:TYR:CE1	1:D:456:VAL:HG22	2.56	0.40
1:A:344:LEU:HB2	1:A:399:TYR:HB2	2.02	0.40
3:L:111:LYS:HA	3:L:142:PRO:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:ASP:HB3	1:D:401:ASN:H	1.86	0.40
3:X:148:TRP:HH2	3:X:176:SER:HB3	1.86	0.40
1:C:381:SER:C	1:C:383:CYS:H	2.24	0.40
3:L:90:GLN:NE2	3:L:93:SER:O	2.48	0.40
3:L:125:GLU:HG2	3:L:130:LYS:O	2.22	0.40
2:E:29:ILE:HD12	2:E:34:TRP:CE2	2.56	0.40
3:Y:138:ASP:HA	3:Y:171:LYS:HB3	2.04	0.40
2:J:51:ILE:HG13	2:J:55:GLY:O	2.21	0.40
2:J:47:TRP:CZ2	2:J:49:GLY:HA2	2.57	0.40
2:J:187:VAL:HG12	2:J:189:VAL:HG13	2.03	0.40
2:F:171:PHE:HE2	3:I:173:ALA:O	2.03	0.40
2:H:186:VAL:HG11	3:L:136:LEU:HD11	2.02	0.40
3:L:150:LYS:HA	3:L:154:SER:O	2.22	0.40
3:Y:35:TRP:HB3	3:Y:73:LEU:HD22	2.04	0.40
1:G:360:MET:HB3	1:G:473:ALA:HA	2.02	0.40
2:J:16:GLU:O	2:J:82(C):VAL:HG22	2.22	0.40
2:J:50:ASN:OD1	2:J:58:ASN:HB2	2.21	0.40
3:X:35:TRP:HB2	3:X:48:ILE:HB	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	173/254 (68%)	148 (86%)	25 (14%)	0	100	100
1	C	173/254 (68%)	142 (82%)	31 (18%)	0	100	100
1	D	173/254 (68%)	151 (87%)	22 (13%)	0	100	100
1	G	173/254 (68%)	153 (88%)	20 (12%)	0	100	100
2	E	210/242 (87%)	195 (93%)	15 (7%)	0	100	100
2	F	210/242 (87%)	198 (94%)	10 (5%)	2 (1%)	13	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	210/242 (87%)	194 (92%)	15 (7%)	1 (0%)	25	63
2	J	210/242 (87%)	198 (94%)	12 (6%)	0	100	100
3	I	208/210 (99%)	194 (93%)	14 (7%)	0	100	100
3	L	208/210 (99%)	195 (94%)	13 (6%)	0	100	100
3	X	208/210 (99%)	196 (94%)	12 (6%)	0	100	100
3	Y	208/210 (99%)	195 (94%)	13 (6%)	0	100	100
All	All	2364/2824 (84%)	2159 (91%)	202 (8%)	3 (0%)	48	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	29	ILE
2	F	151	PHE
2	F	152	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	154/216 (71%)	146 (95%)	8 (5%)	19	42
1	C	154/216 (71%)	144 (94%)	10 (6%)	14	36
1	D	154/216 (71%)	148 (96%)	6 (4%)	27	49
1	G	154/216 (71%)	144 (94%)	10 (6%)	14	36
2	E	184/209 (88%)	182 (99%)	2 (1%)	70	80
2	F	184/209 (88%)	183 (100%)	1 (0%)	86	90
2	H	184/209 (88%)	179 (97%)	5 (3%)	40	60
2	J	184/209 (88%)	180 (98%)	4 (2%)	47	65
3	I	179/179 (100%)	175 (98%)	4 (2%)	47	65
3	L	179/179 (100%)	173 (97%)	6 (3%)	32	53
3	X	179/179 (100%)	177 (99%)	2 (1%)	70	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	Y	179/179 (100%)	175 (98%)	4 (2%)	47 65
All	All	2068/2416 (86%)	2006 (97%)	62 (3%)	36 57

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	314	TRP
1	A	316	TYR
1	A	321	PHE
1	A	325	ASP
1	A	406	ASP
1	A	412	CYS
1	A	470	PHE
1	A	479	PHE
2	H	31	ARG
2	H	52	TYR
2	H	53	TYR
2	H	58	ASN
2	H	151	PHE
3	L	1	ASP
3	L	32	TYR
3	L	139	ASP
3	L	149	TRP
3	L	152	ASP
3	L	187	LYS
1	D	307	ARG
1	D	342	PHE
1	D	383	CYS
1	D	411	TYR
1	D	428	ASP
1	D	479	PHE
2	E	45	LEU
2	E	52	TYR
3	Y	1	ASP
3	Y	32	TYR
3	Y	138	ASP
3	Y	151	ASP
1	G	312	HIS
1	G	342	PHE
1	G	366	CYS
1	G	375	CYS
1	G	378	HIS

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Mol	Chain	Res	Type
1	G	407	ASN
1	G	417	HIS
1	G	437	ASP
1	G	470	PHE
1	G	479	PHE
2	J	45	LEU
2	J	63	LEU
2	J	103	ARG
2	J	153	GLU
3	X	138	ASP
3	X	151	ASP
1	C	316	TYR
1	C	379	MET
1	C	406	ASP
1	C	408	TYR
1	C	418	MET
1	C	422	PHE
1	C	424	LEU
1	C	470	PHE
1	C	477	ARG
1	C	479	PHE
2	F	63	LEU
3	I	32	TYR
3	I	135	LEU
3	I	138	ASP
3	I	151	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	Y	194	GLN
3	Y	197	HIS
2	J	77	GLN
1	C	407	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	175/254 (68%)	0.33	4 (2%) 61 45	17, 60, 133, 174	0
1	C	175/254 (68%)	0.45	8 (4%) 38 31	19, 67, 127, 207	0
1	D	175/254 (68%)	0.45	2 (1%) 77 63	30, 71, 133, 180	0
1	G	175/254 (68%)	0.49	4 (2%) 61 45	31, 75, 127, 169	0
2	E	214/242 (88%)	1.00	23 (10%) 12 13	64, 131, 222, 235	0
2	F	214/242 (88%)	0.37	4 (1%) 66 50	21, 66, 112, 132	0
2	H	214/242 (88%)	0.28	2 (0%) 81 67	24, 72, 111, 134	0
2	J	214/242 (88%)	0.80	9 (4%) 41 32	57, 127, 182, 202	0
3	I	210/210 (100%)	0.37	5 (2%) 59 45	19, 52, 96, 156	0
3	L	210/210 (100%)	0.34	6 (2%) 54 40	19, 53, 97, 128	0
3	X	210/210 (100%)	0.87	18 (8%) 18 17	47, 121, 194, 215	0
3	Y	210/210 (100%)	1.35	44 (20%) 3 5	69, 176, 223, 259	0
All	All	2396/2824 (84%)	0.60	129 (5%) 32 26	17, 82, 198, 259	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	184	GLU	5.3
2	E	142	ALA	4.8
2	E	129	LEU	4.2
2	E	128	PRO	4.1
2	E	217	GLU	4.0
2	J	9	PRO	4.0
3	Y	157	ALA	3.8
1	G	430	GLY	3.7
2	E	146	LEU	3.6
3	Y	112	ALA	3.4
3	X	116	THR	3.3

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Mol	Chain	Res	Type	RSRZ
3	X	185	TRP	3.3
3	Y	181	THR	3.3
3	Y	137	SER	3.2
3	I	107	GLY	3.2
3	Y	172	TYR	3.1
1	C	469	HIS	3.1
3	X	163	THR	3.1
2	J	140	THR	3.1
3	Y	196	THR	3.1
3	Y	209	THR	3.0
3	Y	146	VAL	3.0
3	Y	118	PHE	3.0
3	X	179	SER	3.0
3	Y	144	VAL	3.0
2	E	218	PRO	3.0
1	A	407	ASN	2.9
3	Y	202	VAL	2.9
3	Y	161	THR	2.9
2	J	156	THR	2.9
3	L	201	SER	2.8
3	Y	114	SER	2.8
3	I	83	PHE	2.8
3	Y	158	GLY	2.8
3	X	148	TRP	2.7
3	Y	205	THR	2.7
3	X	207	ALA	2.7
2	F	64	GLN	2.7
3	Y	184	GLN	2.7
3	Y	119	PRO	2.7
1	A	370	PRO	2.6
2	E	117	SER	2.6
2	H	27	GLY	2.6
2	F	117	SER	2.6
1	C	468	ASP	2.6
2	J	7	SER	2.6
3	Y	100	GLY	2.6
2	J	212	VAL	2.6
2	E	196	THR	2.6
3	Y	143	ALA	2.6
3	X	197	HIS	2.6
1	C	406	ASP	2.5
3	Y	135	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
3	X	100	GLY	2.5
2	E	200	ILE	2.5
2	J	194	LEU	2.5
3	Y	145	THR	2.5
3	X	165	SER	2.5
3	Y	180	LEU	2.5
3	Y	168	SER	2.5
3	Y	5	THR	2.5
3	Y	153	SER	2.5
1	C	341	PRO	2.5
3	Y	113	PRO	2.5
2	E	183	LEU	2.4
3	Y	131	THR	2.4
1	G	371	ASN	2.4
3	X	157	ALA	2.4
3	X	205	THR	2.4
2	E	174	VAL	2.4
3	I	182	PRO	2.4
2	E	171	PHE	2.4
3	Y	63	SER	2.4
3	Y	165	SER	2.4
3	Y	187	SER	2.4
3	Y	173	ALA	2.3
3	X	107	GLY	2.3
3	Y	54	LEU	2.3
2	J	131	PRO	2.3
1	C	382	GLY	2.3
1	C	467	VAL	2.3
3	Y	188	HIS	2.3
1	A	379	MET	2.2
2	E	192	SER	2.2
3	X	191	TYR	2.2
2	H	7	SER	2.2
2	E	186	VAL	2.2
3	Y	186	LYS	2.2
3	L	152	ASP	2.2
3	Y	109	PRO	2.2
3	Y	179	SER	2.2
1	D	469	HIS	2.2
3	X	192	SER	2.2
3	Y	197	HIS	2.2
1	D	381	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	121	THR	2.2
3	X	149	LYS	2.2
2	E	178	SER	2.2
3	L	171	ASN	2.1
3	X	7	SER	2.1
3	X	114	SER	2.1
1	G	363	TYR	2.1
3	L	185	GLN	2.1
1	G	347	GLU	2.1
2	E	147	VAL	2.1
2	J	123	GLY	2.1
3	Y	111	ALA	2.1
3	I	152	SER	2.1
3	Y	201	THR	2.1
2	E	190	PRO	2.1
3	Y	7	SER	2.1
3	I	189	ARG	2.1
3	Y	41	GLY	2.1
3	Y	207	ALA	2.1
2	E	157	VAL	2.1
2	F	118	SER	2.1
1	A	469	HIS	2.1
2	E	127	PHE	2.1
2	E	172	PRO	2.1
2	J	139	GLY	2.0
2	F	84	ALA	2.0
3	Y	162	THR	2.0
2	E	163	ALA	2.0
1	C	428	ASP	2.0
2	E	126	VAL	2.0
3	Y	192	SER	2.0
3	X	142	GLY	2.0
3	L	129	ASN	2.0
1	C	378	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.