



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 10:52 AM EDT

PDB ID : 5NAV / pdb_00005nav
Title : Crystal structure of the double mutant (Cys211Ser/Cys292Ser) 6-phospho-b-D-glucosidase from *Lactobacillus plantarum*
Authors : Acebron, I.; Mancheno, J.M.
Deposited on : 2017-02-28
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

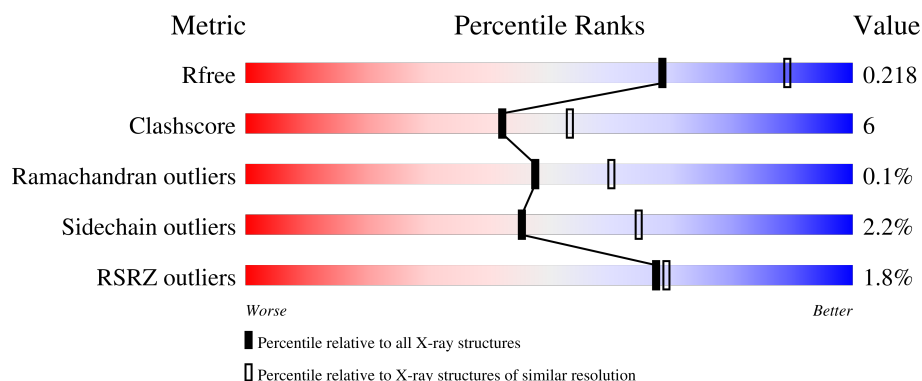
1 Overall quality at a glance

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	477	
1	B	477	
1	C	477	
1	D	477	
1	E	477	

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Mol	Chain	Length	Quality of chain
1	F	477	4% 81% 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24046 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 Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3730	2401	628	685	16			
1	B	461	Total	C	N	O	S	0	0	0
			3730	2401	628	685	16			
1	C	461	Total	C	N	O	S	0	0	0
			3730	2401	628	685	16			
1	D	461	Total	C	N	O	S	0	0	0
			3730	2401	628	685	16			
1	E	461	Total	C	N	O	S	0	0	0
			3730	2401	628	685	16			
1	F	461	Total	C	N	O	S	0	0	0
			3730	2401	628	685	16			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP F9ULH8
A	-14	GLY	-	expression tag	UNP F9ULH8
A	-13	GLY	-	expression tag	UNP F9ULH8
A	-12	SER	-	expression tag	UNP F9ULH8
A	-11	HIS	-	expression tag	UNP F9ULH8
A	-10	HIS	-	expression tag	UNP F9ULH8
A	-9	HIS	-	expression tag	UNP F9ULH8
A	-8	HIS	-	expression tag	UNP F9ULH8
A	-7	HIS	-	expression tag	UNP F9ULH8
A	-6	HIS	-	expression tag	UNP F9ULH8
A	-5	GLY	-	expression tag	UNP F9ULH8
A	-4	ASP	-	expression tag	UNP F9ULH8
A	-3	ASP	-	expression tag	UNP F9ULH8
A	-2	ASP	-	expression tag	UNP F9ULH8
A	-1	ASP	-	expression tag	UNP F9ULH8
A	0	LYS	-	expression tag	UNP F9ULH8
A	211	SER	CYS	engineered mutation	UNP F9ULH8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	292	SER	CYS	engineered mutation	UNP F9ULH8
B	-15	MET	-	initiating methionine	UNP F9ULH8
B	-14	GLY	-	expression tag	UNP F9ULH8
B	-13	GLY	-	expression tag	UNP F9ULH8
B	-12	SER	-	expression tag	UNP F9ULH8
B	-11	HIS	-	expression tag	UNP F9ULH8
B	-10	HIS	-	expression tag	UNP F9ULH8
B	-9	HIS	-	expression tag	UNP F9ULH8
B	-8	HIS	-	expression tag	UNP F9ULH8
B	-7	HIS	-	expression tag	UNP F9ULH8
B	-6	HIS	-	expression tag	UNP F9ULH8
B	-5	GLY	-	expression tag	UNP F9ULH8
B	-4	ASP	-	expression tag	UNP F9ULH8
B	-3	ASP	-	expression tag	UNP F9ULH8
B	-2	ASP	-	expression tag	UNP F9ULH8
B	-1	ASP	-	expression tag	UNP F9ULH8
B	0	LYS	-	expression tag	UNP F9ULH8
B	211	SER	CYS	engineered mutation	UNP F9ULH8
B	292	SER	CYS	engineered mutation	UNP F9ULH8
C	-15	MET	-	initiating methionine	UNP F9ULH8
C	-14	GLY	-	expression tag	UNP F9ULH8
C	-13	GLY	-	expression tag	UNP F9ULH8
C	-12	SER	-	expression tag	UNP F9ULH8
C	-11	HIS	-	expression tag	UNP F9ULH8
C	-10	HIS	-	expression tag	UNP F9ULH8
C	-9	HIS	-	expression tag	UNP F9ULH8
C	-8	HIS	-	expression tag	UNP F9ULH8
C	-7	HIS	-	expression tag	UNP F9ULH8
C	-6	HIS	-	expression tag	UNP F9ULH8
C	-5	GLY	-	expression tag	UNP F9ULH8
C	-4	ASP	-	expression tag	UNP F9ULH8
C	-3	ASP	-	expression tag	UNP F9ULH8
C	-2	ASP	-	expression tag	UNP F9ULH8
C	-1	ASP	-	expression tag	UNP F9ULH8
C	0	LYS	-	expression tag	UNP F9ULH8
C	211	SER	CYS	engineered mutation	UNP F9ULH8
C	292	SER	CYS	engineered mutation	UNP F9ULH8
D	-15	MET	-	initiating methionine	UNP F9ULH8
D	-14	GLY	-	expression tag	UNP F9ULH8
D	-13	GLY	-	expression tag	UNP F9ULH8
D	-12	SER	-	expression tag	UNP F9ULH8
D	-11	HIS	-	expression tag	UNP F9ULH8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	HIS	-	expression tag	UNP F9ULH8
D	-9	HIS	-	expression tag	UNP F9ULH8
D	-8	HIS	-	expression tag	UNP F9ULH8
D	-7	HIS	-	expression tag	UNP F9ULH8
D	-6	HIS	-	expression tag	UNP F9ULH8
D	-5	GLY	-	expression tag	UNP F9ULH8
D	-4	ASP	-	expression tag	UNP F9ULH8
D	-3	ASP	-	expression tag	UNP F9ULH8
D	-2	ASP	-	expression tag	UNP F9ULH8
D	-1	ASP	-	expression tag	UNP F9ULH8
D	0	LYS	-	expression tag	UNP F9ULH8
D	211	SER	CYS	engineered mutation	UNP F9ULH8
D	292	SER	CYS	engineered mutation	UNP F9ULH8
E	-15	MET	-	initiating methionine	UNP F9ULH8
E	-14	GLY	-	expression tag	UNP F9ULH8
E	-13	GLY	-	expression tag	UNP F9ULH8
E	-12	SER	-	expression tag	UNP F9ULH8
E	-11	HIS	-	expression tag	UNP F9ULH8
E	-10	HIS	-	expression tag	UNP F9ULH8
E	-9	HIS	-	expression tag	UNP F9ULH8
E	-8	HIS	-	expression tag	UNP F9ULH8
E	-7	HIS	-	expression tag	UNP F9ULH8
E	-6	HIS	-	expression tag	UNP F9ULH8
E	-5	GLY	-	expression tag	UNP F9ULH8
E	-4	ASP	-	expression tag	UNP F9ULH8
E	-3	ASP	-	expression tag	UNP F9ULH8
E	-2	ASP	-	expression tag	UNP F9ULH8
E	-1	ASP	-	expression tag	UNP F9ULH8
E	0	LYS	-	expression tag	UNP F9ULH8
E	211	SER	CYS	engineered mutation	UNP F9ULH8
E	292	SER	CYS	engineered mutation	UNP F9ULH8
F	-15	MET	-	initiating methionine	UNP F9ULH8
F	-14	GLY	-	expression tag	UNP F9ULH8
F	-13	GLY	-	expression tag	UNP F9ULH8
F	-12	SER	-	expression tag	UNP F9ULH8
F	-11	HIS	-	expression tag	UNP F9ULH8
F	-10	HIS	-	expression tag	UNP F9ULH8
F	-9	HIS	-	expression tag	UNP F9ULH8
F	-8	HIS	-	expression tag	UNP F9ULH8
F	-7	HIS	-	expression tag	UNP F9ULH8
F	-6	HIS	-	expression tag	UNP F9ULH8
F	-5	GLY	-	expression tag	UNP F9ULH8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	ASP	-	expression tag	UNP F9ULH8
F	-3	ASP	-	expression tag	UNP F9ULH8
F	-2	ASP	-	expression tag	UNP F9ULH8
F	-1	ASP	-	expression tag	UNP F9ULH8
F	0	LYS	-	expression tag	UNP F9ULH8
F	211	SER	CYS	engineered mutation	UNP F9ULH8
F	292	SER	CYS	engineered mutation	UNP F9ULH8

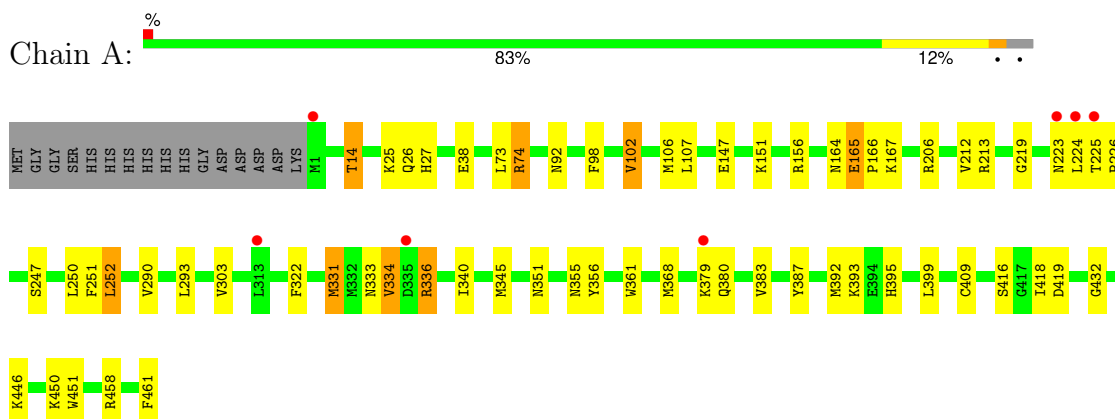
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	360	Total	O	0	0
			360	360		
2	B	263	Total	O	0	0
			263	263		
2	C	311	Total	O	0	0
			311	311		
2	D	248	Total	O	0	0
			248	248		
2	E	299	Total	O	0	0
			299	299		
2	F	185	Total	O	0	0
			185	185		

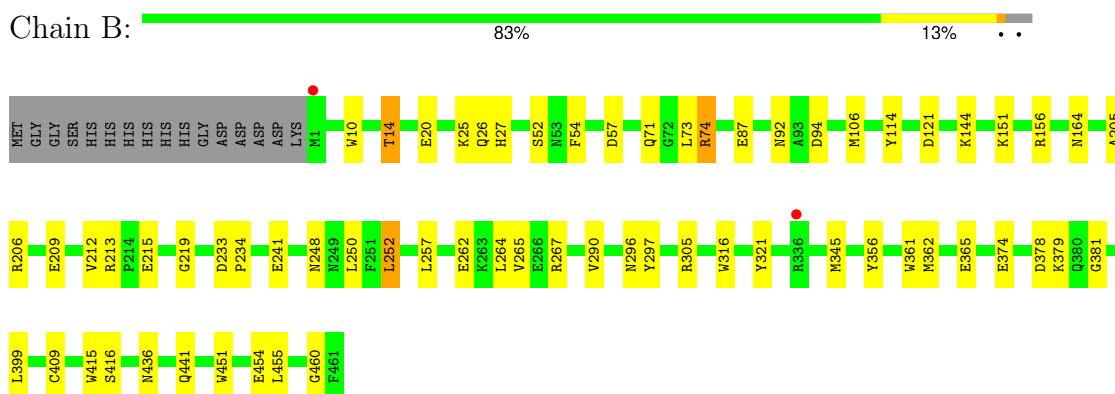
3 Residue-property plots [i](#)

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.

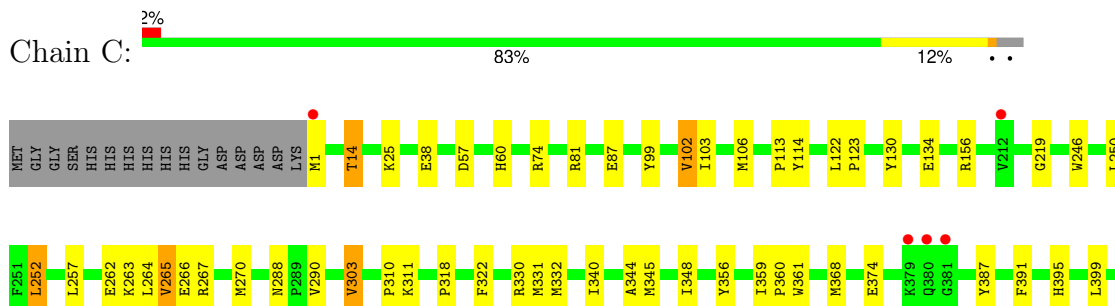
- Molecule 1: Beta-galactosidase

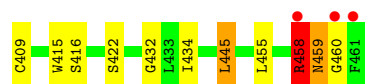


- Molecule 1: Beta-galactosidase

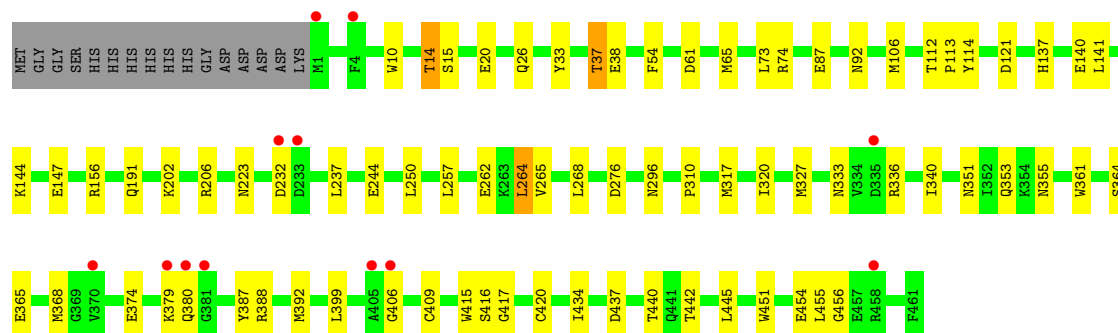
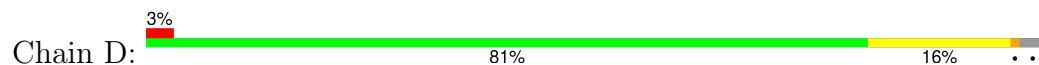


- Molecule 1: Beta-galactosidase

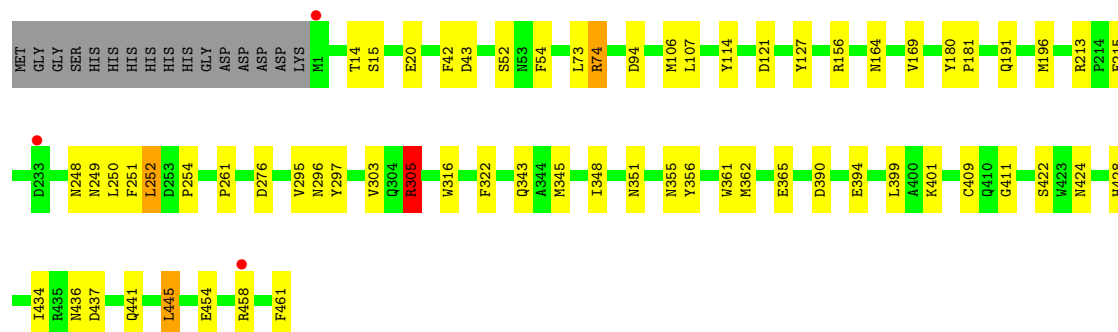
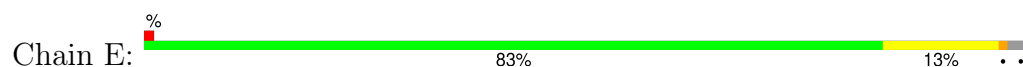




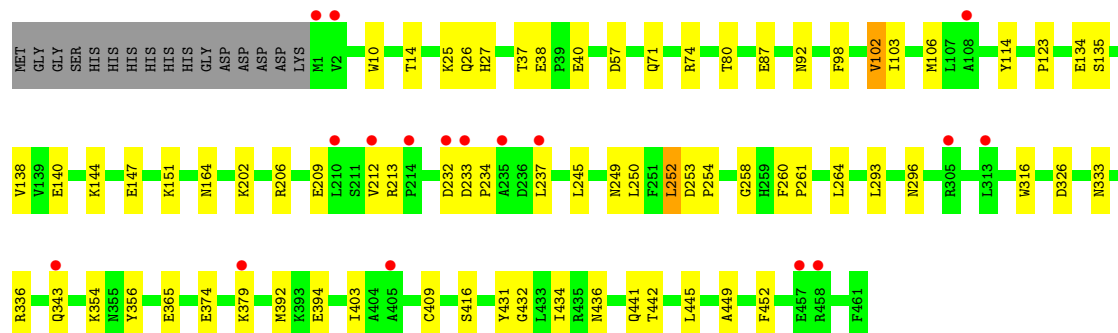
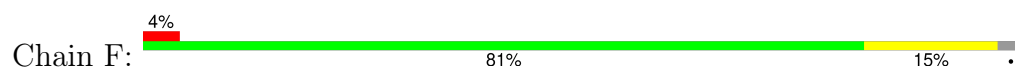
• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	196.74Å 192.06Å 105.84Å 90.00° 102.39° 90.00°	Depositor
Resolution (Å)	38.38 – 2.30 38.38 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.38-2.30) 99.9 (38.38-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.163 , 0.206 0.178 , 0.218	Depositor DCC
R_{free} test set	8504 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24046	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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	0.42	1/3851 (0.0%)	0.59	0/5247
1	B	0.36	0/3851	0.56	0/5247
1	C	0.47	4/3851 (0.1%)	0.61	5/5247 (0.1%)
1	D	0.33	0/3851	0.54	0/5247
1	E	0.38	0/3851	0.55	1/5247 (0.0%)
1	F	0.31	0/3851	0.53	0/5247
All	All	0.39	5/23106 (0.0%)	0.57	6/31482 (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
1	E	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	458	ARG	CZ-NH1	-10.62	1.17	1.32
1	A	165	GLU	C-O	8.38	1.34	1.24
1	C	458	ARG	NE-CZ	-7.25	1.25	1.33
1	C	458	ARG	N-CA	6.47	1.53	1.46
1	C	458	ARG	CB-CG	6.33	1.71	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	458	ARG	CD-NE-CZ	12.48	141.87	124.40
1	C	458	ARG	NE-CZ-NH2	-9.87	110.32	119.20
1	E	305	ARG	NE-CZ-NH2	-7.98	112.02	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	458	ARG	CG-CD-NE	5.58	124.26	112.00
1	C	458	ARG	CB-CG-CD	5.41	123.75	111.30
1	C	458	ARG	NE-CZ-NH1	5.28	126.78	121.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	458	ARG	Mainchain
1	E	305	ARG	Sidechain

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	3730	0	3511	41	0
1	B	3730	0	3511	41	0
1	C	3730	0	3511	47	0
1	D	3730	0	3511	51	0
1	E	3730	0	3511	41	0
1	F	3730	0	3511	54	0
2	A	360	0	0	4	0
2	B	263	0	0	12	0
2	C	311	0	0	12	1
2	D	248	0	0	6	1
2	E	299	0	0	5	0
2	F	185	0	0	13	0
All	All	24046	0	21066	275	1

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 6.

All (275) 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:C:458:ARG:O	1:C:460:GLY:N	1.93	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:TRP:O	2:B:501:HOH:O	1.81	0.99
1:B:374:GLU:OE2	2:B:502:HOH:O	1.81	0.98
1:C:1:MET:N	2:C:502:HOH:O	1.95	0.96
1:A:26:GLN:HE21	1:A:92:ASN:HD22	1.14	0.96
1:A:458:ARG:NH2	2:A:501:HOH:O	1.99	0.95
1:D:191:GLN:HE22	1:D:276:ASP:H	1.07	0.93
1:E:191:GLN:HE22	1:E:276:ASP:H	1.18	0.92
1:F:316:TRP:O	2:F:501:HOH:O	1.88	0.92
1:B:316:TRP:O	2:B:503:HOH:O	1.88	0.91
1:F:37:THR:HG22	1:F:38:GLU:HG3	1.49	0.91
1:C:311:LYS:NZ	2:C:504:HOH:O	2.01	0.91
1:C:310:PRO:O	2:C:501:HOH:O	1.95	0.84
1:A:147:GLU:OE1	1:A:206:ARG:NH1	2.11	0.83
1:E:458:ARG:HH12	1:E:461:PHE:HA	1.44	0.81
1:A:165:GLU:OE2	1:A:223:ASN:ND2	2.14	0.81
1:A:368:MET:SD	2:A:806:HOH:O	2.39	0.81
1:B:94:ASP:HB3	2:B:528:HOH:O	1.80	0.80
1:C:134:GLU:OE2	2:C:503:HOH:O	1.98	0.80
1:B:241:GLU:OE2	2:B:504:HOH:O	2.00	0.79
1:A:38:GLU:OE1	2:A:502:HOH:O	2.01	0.77
1:E:458:ARG:NH1	1:E:461:PHE:HA	2.00	0.77
1:E:305:ARG:NH2	2:E:503:HOH:O	2.18	0.76
1:F:151:LYS:O	2:F:502:HOH:O	2.02	0.76
1:B:248:ASN:ND2	2:B:505:HOH:O	2.20	0.75
1:D:276:ASP:OD1	2:D:501:HOH:O	2.05	0.75
1:F:40:GLU:OE2	2:F:503:HOH:O	2.05	0.75
1:F:374:GLU:OE2	2:F:504:HOH:O	2.05	0.74
1:B:206:ARG:NH2	1:B:209:GLU:OE1	2.20	0.73
1:A:368:MET:HE3	1:A:387:TYR:HD1	1.53	0.73
1:F:394:GLU:OE1	2:F:505:HOH:O	2.06	0.73
1:F:209:GLU:OE1	2:F:506:HOH:O	2.07	0.73
1:C:455:LEU:O	1:C:459:ASN:N	2.22	0.72
1:A:351:ASN:ND2	1:A:355:ASN:HD22	1.88	0.72
1:C:103:ILE:HA	1:C:106:MET:HE2	1.71	0.71
1:C:288:ASN:OD1	2:C:505:HOH:O	2.08	0.71
1:E:454:GLU:HG3	1:E:458:ARG:HE	1.55	0.71
1:A:345:MET:HE2	1:A:395:HIS:HB3	1.72	0.70
1:A:351:ASN:HD22	1:A:355:ASN:HD22	1.39	0.70
1:F:103:ILE:HA	1:F:106:MET:HE3	1.74	0.69
1:A:331:MET:HG2	1:A:340:ILE:HB	1.73	0.69
1:F:26:GLN:HE21	1:F:92:ASN:HD22	1.38	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:212:VAL:HG23	1:F:213:ARG:HG3	1.74	0.69
1:F:38:GLU:OE1	2:F:507:HOH:O	2.11	0.68
1:A:26:GLN:NE2	1:A:92:ASN:HD22	1.88	0.68
1:C:445:LEU:O	2:C:506:HOH:O	2.12	0.67
1:E:248:ASN:ND2	2:E:507:HOH:O	2.28	0.66
1:C:38:GLU:OE1	2:C:508:HOH:O	2.14	0.65
1:C:340:ILE:O	2:C:507:HOH:O	2.14	0.64
1:D:65:MET:HE3	1:D:417:GLY:HA3	1.77	0.64
1:D:437:ASP:HB3	2:D:699:HOH:O	1.96	0.64
1:D:310:PRO:O	2:D:502:HOH:O	2.15	0.64
1:E:316:TRP:O	2:E:502:HOH:O	2.15	0.63
1:B:205:ALA:O	1:B:209:GLU:HG3	1.99	0.63
1:D:380:GLN:OE1	1:D:380:GLN:N	2.32	0.63
1:B:252:LEU:HD13	1:B:356:TYR:CZ	2.33	0.62
1:E:73:LEU:HD23	1:E:106:MET:HE2	1.80	0.62
1:A:379:LYS:HG3	1:A:380:GLN:OE1	2.00	0.62
1:E:297:TYR:HB3	1:E:345:MET:HE2	1.81	0.61
1:A:212:VAL:HG23	1:A:213:ARG:HG3	1.83	0.60
1:D:379:LYS:HD3	1:D:379:LYS:N	2.15	0.60
1:C:103:ILE:HA	1:C:106:MET:CE	2.31	0.60
1:F:232:ASP:C	1:F:237:LEU:HD11	2.27	0.60
1:D:451:TRP:O	1:D:454:GLU:HG3	2.03	0.59
1:A:392:MET:HE2	1:A:451:TRP:CZ3	2.38	0.59
1:C:368:MET:HE3	1:C:387:TYR:HD1	1.68	0.59
1:F:26:GLN:NE2	1:F:92:ASN:HD22	2.01	0.59
1:F:336:ARG:NH2	1:F:431:TYR:OH	2.36	0.58
1:F:392:MET:HE1	1:F:452:PHE:HD1	1.69	0.58
1:D:333:ASN:HB2	1:D:340:ILE:HD11	1.84	0.57
1:B:26:GLN:NE2	1:B:92:ASN:HD22	2.02	0.57
1:F:57:ASP:OD2	2:F:508:HOH:O	2.17	0.57
1:C:391:PHE:O	1:C:395:HIS:HD2	1.86	0.57
1:B:361:TRP:CZ2	1:B:409:CYS:HB2	2.40	0.57
1:A:380:GLN:OE1	1:A:380:GLN:N	2.38	0.57
1:D:244:GLU:OE1	2:D:503:HOH:O	2.18	0.57
1:F:258:GLY:O	2:F:509:HOH:O	2.18	0.56
1:C:57:ASP:OD2	2:C:509:HOH:O	2.17	0.56
1:F:434:ILE:HG12	1:F:445:LEU:HD22	1.87	0.56
1:A:167:LYS:HE3	1:A:247:SER:HA	1.87	0.56
1:F:237:LEU:HD12	1:F:237:LEU:H	1.71	0.56
1:E:436:ASN:HD21	1:E:441:GLN:HE22	1.52	0.55
1:A:147:GLU:HG2	1:A:151:LYS:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:TYR:O	1:D:37:THR:HB	2.07	0.55
1:E:191:GLN:NE2	1:E:276:ASP:H	1.97	0.55
1:F:254:PRO:HG3	1:F:260:PHE:CD2	2.41	0.55
1:A:334:VAL:O	1:A:336:ARG:N	2.38	0.55
1:E:401:LYS:N	1:E:401:LYS:HE2	2.21	0.55
1:C:345:MET:HE2	1:C:395:HIS:O	2.07	0.54
1:B:10:TRP:O	1:B:71:GLN:HB2	2.07	0.54
1:F:252:LEU:HD13	1:F:356:TYR:CZ	2.43	0.54
1:D:74:ARG:HA	1:D:114:TYR:O	2.08	0.54
1:F:252:LEU:HD21	1:F:293:LEU:HD21	1.90	0.53
1:E:52:SER:HA	1:E:441:GLN:HE22	1.74	0.53
1:F:392:MET:HE1	1:F:452:PHE:CD1	2.42	0.53
1:B:305:ARG:NH2	2:B:511:HOH:O	2.39	0.53
1:B:267:ARG:HD2	1:B:321:TYR:OH	2.09	0.53
1:B:26:GLN:HE21	1:B:92:ASN:HD22	1.57	0.52
1:B:73:LEU:HB3	1:B:106:MET:HE3	1.91	0.52
1:C:106:MET:HE1	1:C:113:PRO:HB3	1.90	0.52
1:C:458:ARG:O	1:C:459:ASN:C	2.50	0.52
1:F:436:ASN:HD21	1:F:441:GLN:HA	1.74	0.52
1:B:297:TYR:HB3	1:B:345:MET:HE2	1.90	0.52
1:F:374:GLU:CD	1:F:374:GLU:H	2.17	0.52
1:E:20:GLU:HA	1:E:54:PHE:HB3	1.92	0.52
1:C:395:HIS:HE1	2:C:527:HOH:O	1.93	0.52
1:E:454:GLU:HG3	1:E:458:ARG:NE	2.22	0.52
1:A:14:THR:HG23	1:A:416:SER:OG	2.11	0.51
1:B:455:LEU:N	2:B:501:HOH:O	2.04	0.51
1:C:219:GLY:HA2	1:C:290:VAL:HB	1.92	0.51
1:C:330:ARG:HG3	1:C:332:MET:SD	2.51	0.51
1:A:74:ARG:HH22	1:A:164:ASN:ND2	2.09	0.51
1:C:252:LEU:HD13	1:C:356:TYR:CZ	2.46	0.51
1:D:141:LEU:HD23	1:D:144:LYS:HE3	1.94	0.50
1:A:252:LEU:HD13	1:A:356:TYR:CZ	2.46	0.50
1:C:266:GLU:O	1:C:270:MET:HG3	2.12	0.50
1:B:219:GLY:HA2	1:B:290:VAL:HB	1.94	0.50
1:E:361:TRP:CZ2	1:E:409:CYS:HB2	2.46	0.50
1:A:361:TRP:CZ2	1:A:409:CYS:HB2	2.46	0.50
1:B:74:ARG:HH22	1:B:164:ASN:ND2	2.08	0.50
1:F:74:ARG:HH22	1:F:164:ASN:ND2	2.10	0.50
1:C:345:MET:CE	1:C:399:LEU:HB2	2.41	0.49
1:C:87:GLU:OE1	1:C:130:TYR:OH	2.29	0.49
1:B:378:ASP:OD2	1:B:381:GLY:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:436:ASN:HD21	1:E:441:GLN:NE2	2.09	0.49
1:F:343:GLN:O	1:F:343:GLN:HG2	2.11	0.49
1:F:134:GLU:OE1	2:F:510:HOH:O	2.20	0.49
1:D:434:ILE:HG12	1:D:445:LEU:HD23	1.93	0.49
1:E:303:VAL:HG13	1:E:322:PHE:HB2	1.95	0.49
1:F:253:ASP:HB2	1:F:261:PRO:HD3	1.95	0.49
1:A:166:PRO:HB2	1:A:251:PHE:CE1	2.48	0.49
1:B:262:GLU:HG2	2:B:712:HOH:O	2.12	0.49
1:B:14:THR:HG23	1:B:416:SER:OG	2.12	0.48
1:D:26:GLN:HE21	1:D:92:ASN:HD22	1.60	0.48
1:D:73:LEU:HB3	1:D:106:MET:HE3	1.95	0.48
1:A:219:GLY:HA2	1:A:290:VAL:HB	1.94	0.48
1:C:374:GLU:H	1:C:374:GLU:CD	2.21	0.48
1:A:73:LEU:HD23	1:A:106:MET:HE3	1.95	0.48
1:B:212:VAL:HG23	1:B:213:ARG:HG3	1.96	0.48
1:C:246:TRP:CZ2	1:C:318:PRO:HG3	2.49	0.48
1:D:456:GLY:HA3	2:D:622:HOH:O	2.13	0.48
1:D:336:ARG:O	1:D:336:ARG:HG3	2.14	0.48
1:D:351:ASN:HD22	1:D:355:ASN:HD22	1.60	0.48
1:B:87:GLU:O	1:B:144:LYS:HE3	2.14	0.48
1:D:264:LEU:HD22	1:D:268:LEU:HG	1.96	0.47
1:A:223:ASN:O	1:A:224:LEU:HD23	2.14	0.47
1:B:233:ASP:OD1	1:B:234:PRO:HD2	2.14	0.47
1:B:25:LYS:HE3	1:B:27:HIS:O	2.15	0.47
1:F:403:ILE:HG12	1:F:409:CYS:HB3	1.97	0.47
1:A:383:VAL:HB	1:A:446:LYS:HG2	1.96	0.47
1:D:191:GLN:HE22	1:D:276:ASP:N	1.92	0.47
1:B:114:TYR:CE2	1:B:362:MET:HE1	2.49	0.47
1:D:14:THR:HG23	1:D:416:SER:OG	2.14	0.47
1:E:213:ARG:HB3	1:E:215:GLU:OE2	2.14	0.47
1:F:80:THR:HG22	1:F:123:PRO:HB3	1.97	0.47
1:D:440:THR:OG1	1:D:442:THR:HG23	2.14	0.47
1:F:416:SER:O	1:F:432:GLY:HA2	2.14	0.47
1:F:442:THR:OG1	2:F:511:HOH:O	2.20	0.47
1:E:434:ILE:HG12	1:E:445:LEU:HD22	1.96	0.46
1:F:140:GLU:OE2	1:F:202:LYS:NZ	2.37	0.46
1:D:368:MET:HE2	1:D:368:MET:HB3	1.64	0.46
1:C:416:SER:O	1:C:432:GLY:HA2	2.16	0.46
1:B:151:LYS:O	2:B:506:HOH:O	2.20	0.46
1:B:460:GLY:O	2:B:507:HOH:O	2.20	0.46
1:C:99:TYR:HA	1:C:102:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:GLN:NE2	1:D:92:ASN:HD22	2.14	0.46
1:D:368:MET:HE1	1:D:387:TYR:C	2.40	0.46
1:A:303:VAL:HG13	1:A:322:PHE:HB2	1.97	0.46
1:E:127:TYR:CE2	1:E:181:PRO:HG3	2.51	0.46
1:B:415:TRP:HA	1:B:416:SER:HA	1.68	0.46
1:C:122:LEU:HD12	1:C:123:PRO:HD2	1.98	0.46
1:A:333:ASN:HA	2:A:514:HOH:O	2.15	0.46
1:B:52:SER:HA	1:B:441:GLN:HE22	1.80	0.46
1:B:213:ARG:HB3	1:B:215:GLU:OE2	2.16	0.46
1:B:379:LYS:HB2	1:B:379:LYS:HE2	1.75	0.46
1:C:60:HIS:HD2	2:C:509:HOH:O	1.98	0.46
1:F:102:VAL:HG23	1:F:106:MET:HE2	1.96	0.46
1:B:436:ASN:HD21	1:B:441:GLN:HE22	1.63	0.46
1:C:344:ALA:O	1:C:348:ILE:HG13	2.15	0.46
1:D:262:GLU:O	1:D:265:VAL:HG22	2.15	0.46
1:E:343:GLN:CD	1:E:343:GLN:H	2.23	0.46
1:D:351:ASN:ND2	1:D:355:ASN:HD22	2.13	0.45
1:E:74:ARG:HA	1:E:114:TYR:O	2.16	0.45
1:F:326:ASP:HA	2:F:548:HOH:O	2.16	0.45
1:D:147:GLU:OE1	1:D:206:ARG:NH1	2.50	0.45
1:E:169:VAL:HG21	1:E:196:MET:HE1	1.99	0.45
1:B:296:ASN:CG	1:B:365:GLU:HB2	2.42	0.45
1:D:37:THR:CG2	1:D:38:GLU:HG3	2.47	0.45
1:D:361:TRP:CZ2	1:D:409:CYS:HB2	2.50	0.45
1:D:416:SER:OG	1:D:417:GLY:N	2.49	0.45
1:E:251:PHE:C	1:E:254:PRO:HD2	2.41	0.45
1:F:87:GLU:O	1:F:144:LYS:HE3	2.17	0.45
1:C:303:VAL:HG13	1:C:322:PHE:HB2	1.99	0.44
1:E:437:ASP:HB3	2:E:718:HOH:O	2.16	0.44
1:F:202:LYS:NZ	2:F:527:HOH:O	2.49	0.44
1:B:20:GLU:HA	1:B:54:PHE:HB3	1.98	0.44
1:C:359:ILE:HG13	1:C:360:PRO:HD2	1.99	0.44
1:C:415:TRP:HA	1:C:416:SER:HA	1.80	0.44
1:F:74:ARG:HA	1:F:114:TYR:O	2.16	0.44
1:C:361:TRP:CZ2	1:C:409:CYS:HB2	2.52	0.44
1:D:74:ARG:NH2	1:D:365:GLU:HG3	2.32	0.44
1:D:14:THR:HG22	1:D:420:CYS:SG	2.58	0.44
1:E:390:ASP:O	1:E:394:GLU:HG3	2.17	0.44
1:F:379:LYS:O	1:F:379:LYS:HG3	2.18	0.44
1:B:267:ARG:HD2	1:B:321:TYR:CZ	2.53	0.43
1:D:388:ARG:O	1:D:392:MET:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:GLU:OE1	1:F:206:ARG:NH1	2.51	0.43
1:C:263:LYS:H	1:C:263:LYS:HE2	1.84	0.43
1:D:87:GLU:OE2	1:D:137:HIS:HE1	2.02	0.43
1:F:233:ASP:OD2	1:F:234:PRO:HD2	2.17	0.43
1:E:14:THR:HB	1:E:15:SER:H	1.64	0.43
1:F:147:GLU:HG3	1:F:206:ARG:HG2	2.00	0.43
1:F:254:PRO:HG3	1:F:260:PHE:CE2	2.53	0.43
1:E:401:LYS:HD3	1:E:401:LYS:HA	1.80	0.43
1:F:445:LEU:HD13	1:F:449:ALA:HB1	2.01	0.43
1:A:432:GLY:O	1:A:446:LYS:NZ	2.49	0.43
1:E:296:ASN:CG	1:E:365:GLU:HB2	2.44	0.43
1:E:351:ASN:OD1	1:E:355:ASN:ND2	2.48	0.43
1:B:121:ASP:OD1	1:B:121:ASP:N	2.51	0.43
1:C:263:LYS:H	1:C:263:LYS:CE	2.32	0.43
1:F:25:LYS:HE3	1:F:27:HIS:O	2.19	0.43
1:D:61:ASP:O	1:D:65:MET:HG3	2.18	0.43
1:E:252:LEU:HD13	1:E:356:TYR:CZ	2.54	0.43
1:E:362:MET:HE2	1:E:411:GLY:HA3	2.00	0.43
1:A:450:LYS:HA	1:A:450:LYS:HD2	1.69	0.43
1:A:336:ARG:HA	1:A:336:ARG:HD2	1.90	0.42
1:F:245:LEU:HA	1:F:249:ASN:HB2	2.00	0.42
1:E:121:ASP:OD1	1:E:121:ASP:N	2.53	0.42
1:C:368:MET:HE1	1:C:387:TYR:O	2.18	0.42
1:A:224:LEU:HD11	1:A:293:LEU:HD21	2.01	0.42
1:A:379:LYS:HG3	1:A:380:GLN:CD	2.44	0.42
1:C:25:LYS:HG3	1:C:81:ARG:HB2	2.01	0.42
1:D:121:ASP:OD1	1:D:121:ASP:N	2.52	0.42
1:D:327:MET:HE2	1:D:327:MET:HB3	1.93	0.42
1:D:415:TRP:HA	1:D:416:SER:HA	1.60	0.42
1:F:296:ASN:CG	1:F:365:GLU:HB2	2.44	0.42
1:C:267:ARG:CZ	1:C:270:MET:HE3	2.50	0.42
1:E:42:PHE:CD2	1:E:424:ASN:HA	2.55	0.42
1:E:180:TYR:CG	1:E:181:PRO:HA	2.55	0.42
1:C:434:ILE:HG12	1:C:445:LEU:HD22	2.02	0.42
1:D:317:MET:O	1:D:320:ILE:HG12	2.19	0.42
1:C:106:MET:CE	1:C:113:PRO:HB3	2.50	0.42
1:C:331:MET:HE2	1:C:331:MET:HB2	1.80	0.41
1:F:10:TRP:H	1:F:71:GLN:NE2	2.18	0.41
1:F:354:LYS:HA	1:F:354:LYS:HD3	1.82	0.41
1:D:14:THR:HB	1:D:15:SER:H	1.65	0.41
1:D:112:THR:HA	1:D:113:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:ASP:HA	1:D:237:LEU:HD11	2.02	0.41
1:E:94:ASP:HB3	2:E:504:HOH:O	2.19	0.41
1:B:296:ASN:OD1	1:B:365:GLU:HB2	2.20	0.41
1:A:393:LYS:HG2	1:A:461:PHE:CE1	2.56	0.41
1:D:10:TRP:CZ3	1:D:455:LEU:HD21	2.55	0.41
1:D:296:ASN:ND2	1:D:364:SER:OG	2.53	0.41
1:E:295:VAL:HG11	1:E:348:ILE:HG21	2.02	0.41
1:A:25:LYS:HE3	1:A:27:HIS:O	2.21	0.41
1:B:454:GLU:N	2:B:501:HOH:O	2.54	0.41
1:D:140:GLU:OE1	1:D:202:LYS:HE2	2.21	0.41
1:C:14:THR:HG21	2:C:558:HOH:O	2.21	0.41
1:C:262:GLU:HA	1:C:265:VAL:HG13	2.02	0.41
1:F:98:PHE:O	1:F:102:VAL:HG13	2.21	0.41
1:F:135:SER:HB3	1:F:138:VAL:HG23	2.02	0.41
1:F:249:ASN:HB3	1:F:261:PRO:HG3	2.02	0.40
1:A:225:THR:HA	1:A:226:PRO:HD3	1.90	0.40
1:A:418:ILE:O	1:A:419:ASP:C	2.64	0.40
1:D:20:GLU:HA	1:D:54:PHE:HB3	2.04	0.40
1:E:249:ASN:HB3	1:E:261:PRO:HG3	2.02	0.40
1:A:98:PHE:O	1:A:102:VAL:HG13	2.22	0.40
1:C:74:ARG:HA	1:C:114:TYR:O	2.20	0.40
1:D:374:GLU:H	1:D:374:GLU:CD	2.29	0.40
1:A:147:GLU:CG	1:A:151:LYS:HE2	2.51	0.40
1:D:223:ASN:ND2	2:D:526:HOH:O	2.54	0.40
1:D:353:GLN:NE2	1:D:406:GLY:C	2.79	0.40
1:E:43:ASP:OD1	1:E:428:HIS:HB2	2.22	0.40
1:E:74:ARG:NH2	1:E:164:ASN:OD1	2.55	0.40
1:F:333:ASN:ND2	1:F:336:ARG:HB2	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:652:HOH:O	2:D:711:HOH:O[1_556]	2.04	0.16

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	459/477 (96%)	439 (96%)	19 (4%)	1 (0%)	43	55
1	B	459/477 (96%)	444 (97%)	15 (3%)	0	100	100
1	C	459/477 (96%)	445 (97%)	13 (3%)	1 (0%)	43	55
1	D	459/477 (96%)	445 (97%)	14 (3%)	0	100	100
1	E	459/477 (96%)	445 (97%)	14 (3%)	0	100	100
1	F	459/477 (96%)	444 (97%)	15 (3%)	0	100	100
All	All	2754/2862 (96%)	2662 (97%)	90 (3%)	2 (0%)	48	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	336	ARG
1	C	459	ASN

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	387/400 (97%)	377 (97%)	10 (3%)	40	59
1	B	387/400 (97%)	377 (97%)	10 (3%)	40	59
1	C	387/400 (97%)	376 (97%)	11 (3%)	38	56
1	D	387/400 (97%)	380 (98%)	7 (2%)	51	70
1	E	387/400 (97%)	379 (98%)	8 (2%)	47	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	387/400 (97%)	382 (99%)	5 (1%)	61 77
All	All	2322/2400 (97%)	2271 (98%)	51 (2%)	45 65

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	74	ARG
1	A	102	VAL
1	A	107	LEU
1	A	156	ARG
1	A	250	LEU
1	A	252	LEU
1	A	331	MET
1	A	334	VAL
1	A	399	LEU
1	B	14	THR
1	B	57	ASP
1	B	74	ARG
1	B	156	ARG
1	B	250	LEU
1	B	252	LEU
1	B	257	LEU
1	B	264	LEU
1	B	265	VAL
1	B	399	LEU
1	C	14	THR
1	C	102	VAL
1	C	156	ARG
1	C	250	LEU
1	C	252	LEU
1	C	257	LEU
1	C	264	LEU
1	C	265	VAL
1	C	303	VAL
1	C	422	SER
1	C	445	LEU
1	D	14	THR
1	D	37	THR
1	D	156	ARG
1	D	250	LEU
1	D	257	LEU

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Mol	Chain	Res	Type
1	D	264	LEU
1	D	399	LEU
1	E	74	ARG
1	E	107	LEU
1	E	156	ARG
1	E	250	LEU
1	E	252	LEU
1	E	399	LEU
1	E	422	SER
1	E	445	LEU
1	F	14	THR
1	F	102	VAL
1	F	250	LEU
1	F	252	LEU
1	F	264	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	28	GLN
1	A	131	HIS
1	A	137	HIS
1	A	164	ASN
1	A	195	ASN
1	A	351	ASN
1	A	366	ASN
1	A	410	GLN
1	A	429	ASN
1	B	26	GLN
1	B	28	GLN
1	B	60	HIS
1	B	78	GLN
1	B	116	ASN
1	B	164	ASN
1	B	208	HIS
1	B	248	ASN
1	B	441	GLN
1	C	18	GLN
1	C	71	GLN
1	C	217	GLN
1	C	248	ASN

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Mol	Chain	Res	Type
1	C	288	ASN
1	C	351	ASN
1	C	355	ASN
1	C	366	ASN
1	C	395	HIS
1	C	408	ASN
1	C	441	GLN
1	D	26	GLN
1	D	28	GLN
1	D	41	GLN
1	D	60	HIS
1	D	78	GLN
1	D	131	HIS
1	D	137	HIS
1	D	191	GLN
1	D	223	ASN
1	D	296	ASN
1	D	304	GLN
1	D	355	ASN
1	D	384	GLN
1	E	18	GLN
1	E	41	GLN
1	E	60	HIS
1	E	116	ASN
1	E	191	GLN
1	E	248	ASN
1	E	353	GLN
1	E	441	GLN
1	F	26	GLN
1	F	53	ASN
1	F	56	ASN
1	F	71	GLN
1	F	78	GLN
1	F	137	HIS
1	F	164	ASN
1	F	249	ASN
1	F	314	GLN
1	F	333	ASN
1	F	366	ASN
1	F	436	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

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	461/477 (96%)	-0.48	7 (1%) 72 73	19, 29, 51, 87	0
1	B	461/477 (96%)	-0.35	2 (0%) 88 89	23, 34, 58, 86	0
1	C	461/477 (96%)	-0.21	8 (1%) 69 70	22, 33, 51, 89	0
1	D	461/477 (96%)	0.37	12 (2%) 57 59	25, 40, 62, 97	0
1	E	461/477 (96%)	-0.06	3 (0%) 84 85	24, 35, 54, 78	0
1	F	461/477 (96%)	0.50	17 (3%) 45 48	24, 44, 67, 91	0
All	All	2766/2862 (96%)	-0.04	49 (1%) 67 69	19, 35, 60, 97	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	460	GLY	5.3
1	C	458	ARG	5.0
1	A	335	ASP	4.1
1	D	1	MET	4.1
1	A	223	ASN	4.0
1	F	1	MET	3.9
1	B	1	MET	3.5
1	F	212	VAL	3.4
1	F	379	LYS	3.4
1	A	225	THR	3.3
1	F	313	LEU	3.2
1	A	1	MET	3.0
1	D	380	GLN	3.0
1	F	232	ASP	3.0
1	C	461	PHE	2.8
1	C	212	VAL	2.8
1	D	381	GLY	2.8
1	D	335	ASP	2.7
1	E	458	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	379	LYS	2.7
1	F	214	PRO	2.6
1	F	458	ARG	2.6
1	A	379	LYS	2.6
1	F	343	GLN	2.5
1	E	1	MET	2.5
1	D	4	PHE	2.4
1	D	370	VAL	2.4
1	D	379	LYS	2.4
1	F	237	LEU	2.4
1	D	233	ASP	2.3
1	F	210	LEU	2.3
1	F	457	GLU	2.3
1	A	224	LEU	2.3
1	D	405	ALA	2.3
1	D	458	ARG	2.2
1	C	380	GLN	2.2
1	D	232	ASP	2.2
1	C	381	GLY	2.2
1	F	305	ARG	2.2
1	C	1	MET	2.2
1	F	235	ALA	2.2
1	F	233	ASP	2.1
1	E	233	ASP	2.1
1	D	406	GLY	2.1
1	F	108	ALA	2.1
1	F	2	VAL	2.1
1	F	405	ALA	2.0
1	A	313	LEU	2.0
1	B	336	ARG	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.