



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:04 PM UTC

PDB ID : 2ZWO / pdb_00002zwo
Title : Crystal structure of Ca2 site mutant of Pro-S324A
Authors : Takeuchi, Y.; Tanaka, S.; Matsumura, H.; Koga, Y.; Takano, K.; Kanaya, S.
Deposited on : 2008-12-17
Resolution : 2.07 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

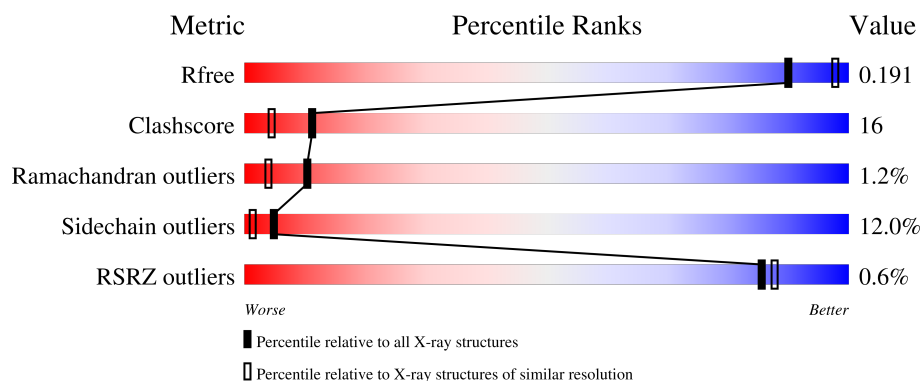
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	398	 67% 26% 7% ..
1	B	398	 64% 27% 7% ..
1	C	398	 59% 30% 8% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9389 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 Tk-subtilisin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			2890	1830	484	569	7			
1	B	393	Total	C	N	O	S	0	0	0
			2888	1828	483	570	7			
1	C	389	Total	C	N	O	S	0	0	0
			2857	1811	478	561	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	226	ALA	ASP	engineered mutation	UNP P58502
A	324	ALA	SER	engineered mutation	UNP P58502
B	226	ALA	ASP	engineered mutation	UNP P58502
B	324	ALA	SER	engineered mutation	UNP P58502
C	226	ALA	ASP	engineered mutation	UNP P58502
C	324	ALA	SER	engineered mutation	UNP P58502

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	Ca	0	0
			6	6		
2	B	5	Total	Ca	0	0
			5	5		
2	C	5	Total	Ca	0	0
			5	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	267	Total	O	0	0
			267	267		

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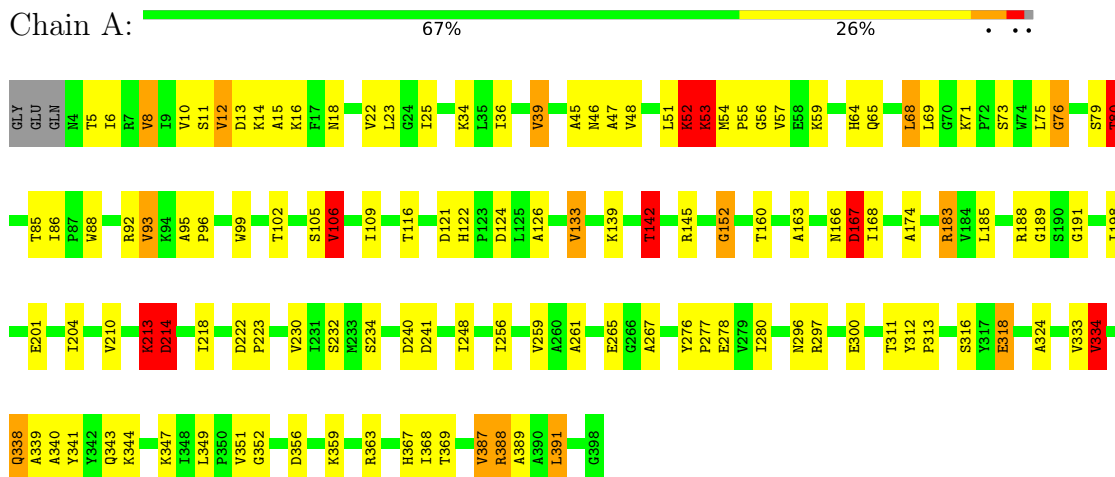
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	251	Total 251	O 251	0	0
3	C	220	Total 220	O 220	0	0

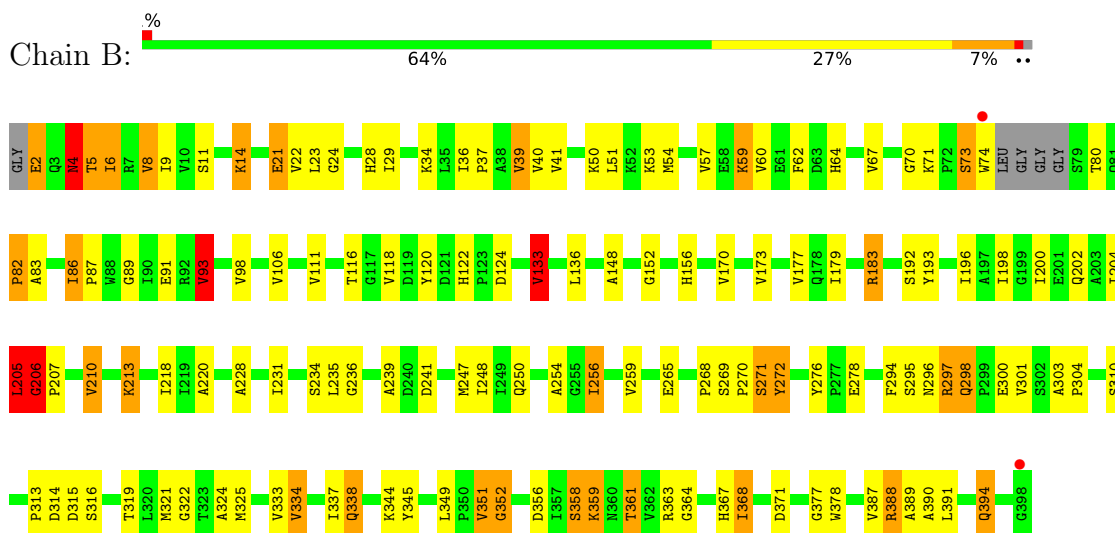
3 Residue-property plots

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: Tk-subtilisin

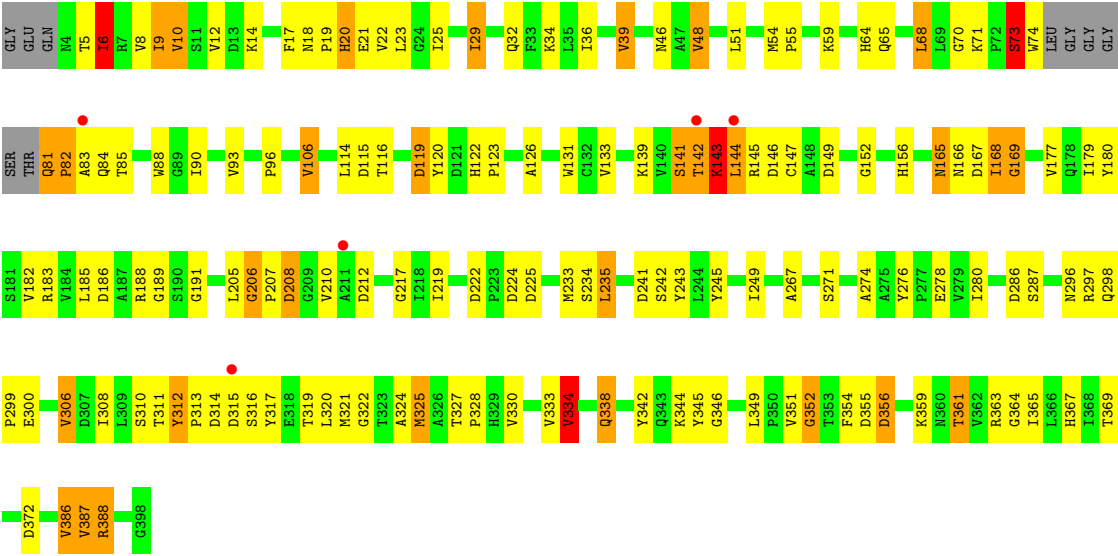


• Molecule 1: Tk-subtilisin



• Molecule 1: Tk-subtilisin





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.73Å 118.31Å 120.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.63 – 2.07 46.63 – 2.07	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.63-2.07) 96.4 (46.63-2.07)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.184 , 0.227 0.185 , 0.191	Depositor DCC
R_{free} test set	3973 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9389	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	1.29	10/2951 (0.3%)	1.37	31/4038 (0.8%)
1	B	1.23	4/2948 (0.1%)	1.34	29/4033 (0.7%)
1	C	1.29	7/2917 (0.2%)	1.41	26/3991 (0.7%)
All	All	1.27	21/8816 (0.2%)	1.37	86/12062 (0.7%)

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	A	0	14
1	B	0	7
1	C	1	10
All	All	1	31

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	210	VAL	C-O	9.18	1.33	1.24
1	C	39	VAL	CA-CB	6.80	1.64	1.54
1	A	174	ALA	CA-CB	6.72	1.61	1.53
1	C	6	ILE	CA-CB	6.33	1.63	1.54
1	A	126	ALA	CA-CB	-6.23	1.43	1.53
1	B	256	ILE	CA-C	6.18	1.59	1.52
1	A	389	ALA	CA-CB	6.16	1.62	1.53
1	C	219	ILE	CA-CB	6.14	1.62	1.54
1	A	334	VAL	CA-CB	5.99	1.61	1.54
1	A	311	THR	CA-C	5.69	1.59	1.52
1	A	39	VAL	CA-CB	5.52	1.62	1.54
1	B	198	ILE	CA-CB	5.48	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	115	ASP	C-O	5.48	1.28	1.24
1	C	276	TYR	N-CA	5.37	1.53	1.45
1	B	301	VAL	N-CA	-5.33	1.39	1.46
1	C	280	ILE	CA-CB	5.31	1.59	1.53
1	C	10	VAL	C-O	-5.20	1.18	1.24
1	A	280	ILE	CA-CB	5.07	1.59	1.53
1	A	36	ILE	CA-CB	5.07	1.60	1.54
1	A	232	SER	N-CA	-5.04	1.40	1.46
1	A	259	VAL	C-O	-5.03	1.18	1.24

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	312	TYR	CA-C-N	-9.63	110.99	120.52
1	C	312	TYR	C-N-CA	-9.63	110.99	120.52
1	C	334	VAL	N-CA-C	9.11	119.91	110.62
1	C	73	SER	N-CA-C	9.09	122.88	111.69
1	A	80	THR	N-CA-C	-8.80	102.28	113.72
1	C	351	VAL	CA-C-N	-8.18	105.38	121.41
1	C	351	VAL	C-N-CA	-8.18	105.38	121.41
1	B	93	VAL	N-CA-C	-8.06	104.71	112.29
1	C	14	LYS	N-CA-C	-7.82	103.72	113.18
1	C	142	THR	N-CA-C	-7.74	94.31	110.80
1	C	36	ILE	N-CA-C	-7.69	102.89	109.19
1	B	206	GLY	CA-C-N	7.64	127.35	119.56
1	B	206	GLY	C-N-CA	7.64	127.35	119.56
1	A	214	ASP	N-CA-C	-7.45	103.32	114.64
1	A	334	VAL	N-CA-C	7.05	117.81	110.62
1	B	204	ILE	N-CA-C	6.96	117.75	110.72
1	A	106	VAL	CB-CA-C	6.95	120.19	111.15
1	A	334	VAL	N-CA-CB	6.77	119.75	110.54
1	B	334	VAL	N-CA-C	6.70	117.45	110.62
1	A	359	LYS	N-CA-C	-6.65	105.04	113.02
1	C	351	VAL	N-CA-C	-6.65	100.17	109.21
1	C	85	THR	N-CA-C	-6.47	99.36	109.72
1	A	312	TYR	CA-C-N	-6.46	113.33	119.85
1	A	312	TYR	C-N-CA	-6.46	113.33	119.85
1	B	54	MET	CA-C-N	-6.39	113.40	119.85
1	B	54	MET	C-N-CA	-6.39	113.40	119.85
1	A	343	GLN	N-CA-C	-6.35	104.44	111.36
1	B	133	VAL	CB-CA-C	-6.32	101.47	110.82
1	C	168	ILE	N-CA-C	6.28	118.21	109.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	298	GLN	CA-C-N	-6.22	112.06	119.84
1	B	298	GLN	C-N-CA	-6.22	112.06	119.84
1	A	71	LYS	N-CA-C	-6.16	101.11	108.25
1	A	160	THR	N-CA-C	6.14	118.77	111.33
1	A	142	THR	N-CA-C	-6.13	103.89	113.02
1	C	224	ASP	N-CA-C	6.00	120.46	113.20
1	A	163	ALA	N-CA-C	-5.97	102.23	110.35
1	B	272	TYR	N-CA-C	5.94	117.55	110.07
1	A	340	ALA	N-CA-C	-5.93	104.90	111.36
1	C	278	GLU	N-CA-C	5.93	120.12	113.01
1	A	133	VAL	CB-CA-C	-5.92	101.71	110.82
1	C	6	ILE	CA-CB-CG2	5.88	120.50	110.50
1	A	152	GLY	N-CA-C	-5.88	107.29	113.58
1	B	205	LEU	N-CA-C	5.87	118.63	111.82
1	A	18	ASN	CA-C-N	5.84	125.70	119.28
1	A	18	ASN	C-N-CA	5.84	125.70	119.28
1	B	256	ILE	N-CA-C	5.83	116.59	108.89
1	C	351	VAL	O-C-N	-5.80	115.87	122.72
1	C	29	ILE	CB-CA-C	5.74	117.89	111.80
1	B	173	VAL	CB-CA-C	-5.71	104.55	112.04
1	B	239	ALA	N-CA-C	5.70	118.10	110.35
1	A	93	VAL	CG1-CB-CG2	5.64	123.22	110.80
1	C	206	GLY	CA-C-N	5.59	125.69	119.32
1	C	206	GLY	C-N-CA	5.59	125.69	119.32
1	A	85	THR	CA-C-N	-5.59	116.48	122.85
1	A	85	THR	C-N-CA	-5.59	116.48	122.85
1	A	45	ALA	N-CA-C	5.57	120.56	111.37
1	C	387	VAL	CG1-CB-CG2	5.53	122.97	110.80
1	C	165	ASN	N-CA-C	5.52	117.29	108.41
1	A	92	ARG	N-CA-C	5.50	118.03	111.71
1	B	34	LYS	N-CA-C	5.46	116.91	111.07
1	B	40	VAL	N-CA-C	5.41	115.98	108.84
1	C	334	VAL	N-CA-CB	5.39	117.87	110.54
1	B	337	ILE	CB-CA-C	-5.37	104.94	111.87
1	B	24	GLY	N-CA-C	5.36	118.72	112.50
1	C	325	MET	CG-SD-CE	-5.29	89.26	100.90
1	B	205	LEU	CA-C-N	5.28	130.16	121.87
1	B	205	LEU	C-N-CA	5.28	130.16	121.87
1	B	250	GLN	N-CA-C	5.27	117.43	111.11
1	A	109	ILE	N-CA-C	5.26	116.27	108.23
1	A	52	LYS	N-CA-C	5.26	122.00	110.80
1	A	368	ILE	N-CA-C	5.24	117.64	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	86	ILE	CA-C-N	-5.23	113.30	119.84
1	B	86	ILE	C-N-CA	-5.23	113.30	119.84
1	A	8	VAL	N-CA-C	-5.22	100.95	108.42
1	A	53	LYS	N-CA-C	5.22	116.71	110.44
1	C	243	TYR	N-CA-C	5.19	116.94	111.28
1	C	90	ILE	N-CA-C	5.16	116.51	110.62
1	A	351	VAL	CA-C-N	-5.13	111.35	121.41
1	A	351	VAL	C-N-CA	-5.13	111.35	121.41
1	B	57	VAL	N-CA-C	5.12	115.60	108.84
1	B	276	TYR	N-CA-C	5.10	116.12	109.64
1	B	351	VAL	CA-C-N	-5.10	111.41	121.41
1	B	351	VAL	C-N-CA	-5.10	111.41	121.41
1	A	351	VAL	O-C-N	-5.08	117.25	122.63
1	B	270	PRO	N-CA-C	5.03	119.38	111.38
1	C	386	VAL	N-CA-C	5.01	115.79	108.58

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	6	ILE	CB

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	VAL	Peptide,Mainchain
1	A	12	VAL	Peptide
1	A	166	ASN	Mainchain
1	A	167	ASP	Peptide,Mainchain
1	A	213	LYS	Peptide
1	A	214	ASP	Peptide
1	A	53	LYS	Peptide
1	A	55	PRO	Peptide
1	A	65	GLN	Mainchain
1	A	75	LEU	Peptide
1	A	76	GLY	Peptide
1	A	79	SER	Peptide
1	B	106	VAL	Peptide
1	B	133	VAL	Mainchain
1	B	205	LEU	Peptide,Mainchain
1	B	259	VAL	Mainchain
1	B	271	SER	Mainchain
1	B	4	ASN	Mainchain

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Mol	Chain	Res	Type	Group
1	C	106	VAL	Peptide
1	C	12	VAL	Peptide
1	C	141	SER	Peptide
1	C	143	LYS	Peptide
1	C	165	ASN	Peptide
1	C	179	ILE	Peptide
1	C	346	GLY	Peptide
1	C	352	GLY	Peptide
1	C	82	PRO	Peptide,Mainchain

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	2890	0	2851	70	0
1	B	2888	0	2844	108	0
1	C	2857	0	2818	109	0
2	A	6	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	267	0	0	7	1
3	B	251	0	0	12	1
3	C	220	0	0	3	2
All	All	9389	0	8513	279	2

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 16.

All (279) 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:B:70:GLY:CA	1:B:325:MET:HE1	1.75	1.16
1:B:338:GLN:HE21	1:B:338:GLN:HA	1.05	1.10
1:B:70:GLY:HA3	1:B:325:MET:HE1	1.34	1.09
1:C:321:MET:C	1:C:325:MET:HE3	1.83	1.04
1:C:361:THR:HG22	1:C:364:GLY:H	1.21	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:MET:C	1:C:325:MET:CE	2.33	1.02
1:B:352:GLY:HA3	1:B:363:ARG:HB2	1.41	0.98
1:A:352:GLY:HA3	1:A:363:ARG:HB2	1.51	0.91
1:B:321:MET:C	1:B:325:MET:HE2	1.95	0.91
1:B:70:GLY:HA2	1:B:325:MET:HE1	1.51	0.90
1:B:361:THR:HG22	1:B:364:GLY:H	1.35	0.90
1:A:122:HIS:HD2	1:A:124:ASP:H	1.17	0.88
1:B:344:LYS:HE2	1:B:345:TYR:OH	1.75	0.85
1:B:338:GLN:HA	1:B:338:GLN:NE2	1.87	0.85
1:C:122:HIS:HE1	1:C:316:SER:O	1.59	0.84
1:B:394:GLN:NE2	3:B:519:HOH:O	2.13	0.81
1:B:371:ASP:HB2	1:B:388:ARG:HD2	1.62	0.80
1:A:210:VAL:O	3:A:514:HOH:O	2.00	0.80
1:B:361:THR:CG2	1:B:364:GLY:H	1.94	0.79
1:B:2:GLU:N	3:B:746:HOH:O	2.15	0.79
1:B:338:GLN:HE21	1:B:338:GLN:CA	1.89	0.79
1:B:356:ASP:OD1	1:B:361:THR:HG21	1.83	0.79
1:B:321:MET:C	1:B:325:MET:CE	2.56	0.78
1:A:25:ILE:CD1	1:A:47:ALA:HB1	2.13	0.78
1:C:361:THR:CG2	1:C:364:GLY:H	1.96	0.78
1:A:356:ASP:O	1:A:367:HIS:HD2	1.65	0.77
1:B:359:LYS:HE2	1:B:368:ILE:HD13	1.67	0.77
1:B:265:GLU:H	1:B:296:ASN:HD21	1.33	0.77
1:C:338:GLN:HE21	1:C:338:GLN:HA	1.50	0.77
1:A:188:ARG:HD2	3:A:639:HOH:O	1.84	0.76
1:A:88:TRP:H	1:B:4:ASN:HD22	1.33	0.76
1:C:352:GLY:CA	1:C:361:THR:HG23	2.17	0.75
1:C:361:THR:HG22	1:C:364:GLY:N	2.01	0.74
1:A:167:ASP:HB3	1:A:168:ILE:HG23	1.69	0.73
1:A:338:GLN:HE21	1:A:338:GLN:HA	1.54	0.73
1:B:344:LYS:HE2	1:B:345:TYR:CZ	2.25	0.72
1:A:25:ILE:HD12	1:A:47:ALA:HB1	1.70	0.71
1:C:300:GLU:OE2	1:C:367:HIS:HE1	1.72	0.71
1:A:106:VAL:HG13	1:A:339:ALA:HB1	1.72	0.71
1:C:321:MET:O	1:C:325:MET:CE	2.38	0.70
1:A:300:GLU:OE2	1:A:367:HIS:HE1	1.75	0.69
1:B:338:GLN:HE22	1:B:349:LEU:H	1.40	0.69
1:C:338:GLN:HE22	1:C:349:LEU:H	1.39	0.69
1:C:233:MET:HB3	1:C:235:LEU:HD22	1.73	0.68
1:C:356:ASP:O	1:C:367:HIS:HD2	1.75	0.68
1:C:122:HIS:CE1	1:C:316:SER:O	2.45	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LYS:O	1:A:52:LYS:HD3	1.93	0.68
1:C:321:MET:O	1:C:325:MET:HE1	1.94	0.68
1:C:352:GLY:HA3	1:C:361:THR:HG23	1.76	0.67
1:C:321:MET:CA	1:C:325:MET:HE3	2.24	0.67
1:A:265:GLU:H	1:A:296:ASN:HD21	1.42	0.67
1:B:36:ILE:HD13	1:B:247:MET:HE2	1.76	0.67
1:C:267:ALA:H	1:C:296:ASN:ND2	1.92	0.66
1:A:64:HIS:HD2	1:A:241:ASP:OD2	1.78	0.66
1:A:69:LEU:HD12	1:A:261:ALA:HB3	1.78	0.66
1:C:122:HIS:CD2	1:C:123:PRO:HD2	2.31	0.65
1:B:300:GLU:OE2	1:B:367:HIS:HE1	1.80	0.65
1:A:218:ILE:HG22	1:A:222:ASP:HB2	1.79	0.65
1:B:356:ASP:OD2	1:B:358:SER:OG	2.13	0.65
3:A:530:HOH:O	1:B:2:GLU:HG3	1.97	0.65
1:C:83:ALA:HB3	1:C:168:ILE:HA	1.79	0.65
1:B:361:THR:HG22	1:B:364:GLY:N	2.09	0.64
1:A:276:TYR:O	3:A:729:HOH:O	2.15	0.64
1:B:321:MET:O	1:B:325:MET:CE	2.46	0.64
1:C:81:GLN:HG2	1:C:82:PRO:HD2	1.78	0.64
1:B:356:ASP:O	1:B:367:HIS:HD2	1.80	0.63
1:A:122:HIS:CD2	1:A:124:ASP:H	2.09	0.62
1:B:21:GLU:HG2	3:B:602:HOH:O	1.99	0.62
1:C:352:GLY:HA3	1:C:363:ARG:HB2	1.80	0.61
1:B:122:HIS:HD2	1:B:124:ASP:H	1.48	0.61
1:C:70:GLY:HA2	1:C:325:MET:HE1	1.80	0.61
1:C:6:ILE:HD11	1:C:48:VAL:CG2	2.30	0.61
1:C:120:TYR:OH	1:C:144:LEU:HD23	2.00	0.60
1:C:300:GLU:OE2	1:C:367:HIS:CE1	2.54	0.59
1:C:34:LYS:HD2	1:C:205:LEU:HD11	1.83	0.59
1:B:116:THR:O	1:B:183:ARG:HD3	2.02	0.59
1:B:122:HIS:HE1	1:B:316:SER:O	1.85	0.59
1:A:116:THR:O	1:A:183:ARG:HD3	2.03	0.58
1:A:25:ILE:HD13	1:A:47:ALA:HB1	1.83	0.58
1:B:322:GLY:N	1:B:325:MET:HE2	2.18	0.57
1:B:152:GLY:HA2	1:B:313:PRO:CD	2.36	0.56
1:B:265:GLU:HB2	3:B:735:HOH:O	2.04	0.56
1:C:267:ALA:H	1:C:296:ASN:HD22	1.54	0.56
1:A:68:LEU:HD13	1:A:189:GLY:HA3	1.88	0.56
1:A:356:ASP:O	1:A:367:HIS:CD2	2.53	0.56
1:B:29:ILE:HG23	1:B:39:VAL:CG2	2.35	0.56
1:A:318:GLU:HG2	1:C:46:ASN:OD1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LEU:HD23	1:A:191:GLY:HA3	1.88	0.56
1:B:265:GLU:CB	3:B:735:HOH:O	2.54	0.56
1:C:9:ILE:N	1:C:9:ILE:HD12	2.21	0.55
1:A:267:ALA:H	1:A:296:ASN:ND2	2.03	0.55
1:B:8:VAL:CG1	1:B:60:VAL:HG13	2.36	0.55
1:A:318:GLU:HG3	3:A:721:HOH:O	2.07	0.55
1:A:265:GLU:H	1:A:296:ASN:ND2	2.03	0.55
1:A:352:GLY:CA	1:A:363:ARG:HB2	2.32	0.55
1:A:11:SER:HB2	1:A:59:LYS:HB3	1.88	0.54
1:A:369:THR:O	1:A:388:ARG:HD3	2.08	0.54
1:C:119:ASP:HB2	1:C:313:PRO:HB3	1.89	0.54
1:B:236:GLY:HA2	1:B:272:TYR:O	2.07	0.54
1:B:50:LYS:HE2	3:B:584:HOH:O	2.07	0.54
1:A:88:TRP:H	1:B:4:ASN:ND2	2.04	0.54
1:A:318:GLU:HG2	1:C:46:ASN:CG	2.32	0.54
1:A:25:ILE:HD12	1:A:47:ALA:CB	2.37	0.54
1:C:6:ILE:HD11	1:C:48:VAL:HG23	1.90	0.54
1:A:25:ILE:HG12	1:A:54:MET:HE1	1.89	0.54
1:B:394:GLN:NE2	1:B:394:GLN:HA	2.23	0.54
1:A:13:ASP:OD1	1:A:15:ALA:HB3	2.08	0.53
1:B:202:GLN:O	1:B:206:GLY:HA2	2.08	0.53
1:A:121:ASP:OD2	1:A:121:ASP:C	2.51	0.53
1:B:11:SER:HB2	1:B:59:LYS:CB	2.39	0.53
1:C:212:ASP:OD2	1:C:217:GLY:N	2.37	0.53
1:C:352:GLY:HA3	1:C:361:THR:CG2	2.39	0.53
1:B:278:GLU:N	1:B:278:GLU:OE1	2.41	0.53
1:B:28:HIS:HB3	3:B:484:HOH:O	2.08	0.52
1:C:114:LEU:HA	1:C:182:VAL:O	2.08	0.52
1:C:352:GLY:CA	1:C:361:THR:CG2	2.87	0.52
1:B:265:GLU:H	1:B:296:ASN:ND2	2.04	0.52
1:C:314:ASP:O	1:C:315:ASP:C	2.52	0.52
1:B:296:ASN:N	1:B:296:ASN:HD22	2.07	0.52
1:C:120:TYR:CZ	1:C:144:LEU:HD23	2.45	0.52
1:A:341:TYR:HD2	1:A:347:LYS:O	1.92	0.52
1:B:170:VAL:HG21	1:B:310:SER:HA	1.92	0.51
1:C:73:SER:CB	1:C:319:THR:HG22	2.40	0.51
1:A:300:GLU:OE2	1:A:367:HIS:CE1	2.62	0.51
1:B:356:ASP:O	1:B:367:HIS:CD2	2.63	0.51
1:C:169:GLY:HA3	1:C:317:TYR:CZ	2.46	0.51
1:C:245:TYR:CZ	1:C:249:ILE:HD11	2.46	0.51
1:B:352:GLY:CA	1:B:363:ARG:HB2	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:ASP:CG	1:B:361:THR:HG21	2.35	0.51
1:B:70:GLY:HA2	1:B:325:MET:CE	2.33	0.51
1:B:205:LEU:O	1:B:210:VAL:O	2.29	0.51
1:A:338:GLN:HE22	1:A:349:LEU:HB2	1.75	0.51
1:B:344:LYS:CE	1:B:345:TYR:OH	2.55	0.51
1:C:286:ASP:HA	1:C:306:VAL:HG13	1.92	0.51
1:A:338:GLN:HE22	1:A:349:LEU:H	1.58	0.51
1:B:8:VAL:HG13	1:B:60:VAL:HG13	1.93	0.51
1:A:167:ASP:CB	1:A:168:ILE:HG23	2.40	0.50
1:C:354:PHE:C	1:C:354:PHE:CD2	2.89	0.50
1:B:14:LYS:HE2	1:B:37:PRO:HA	1.92	0.50
1:B:70:GLY:HA3	1:B:325:MET:CE	2.25	0.50
1:A:10:VAL:HG13	1:A:57:VAL:HG13	1.94	0.50
1:C:64:HIS:HD2	1:C:241:ASP:OD2	1.94	0.50
1:C:344:LYS:HD3	1:C:345:TYR:CE1	2.46	0.50
1:B:98:VAL:CG2	1:B:390:ALA:HA	2.42	0.50
1:B:321:MET:N	1:B:325:MET:HE3	2.26	0.50
1:B:86:ILE:O	1:B:87:PRO:C	2.52	0.49
1:C:322:GLY:N	1:C:325:MET:CE	2.74	0.49
1:A:122:HIS:HE1	1:A:316:SER:O	1.95	0.49
1:C:21:GLU:OE2	1:C:55:PRO:HD2	2.11	0.49
1:C:114:LEU:N	1:C:114:LEU:HD12	2.27	0.49
1:C:312:TYR:CD2	1:C:313:PRO:CD	2.95	0.49
1:C:152:GLY:HA2	1:C:313:PRO:CG	2.42	0.49
1:B:303:ALA:HB1	1:B:304:PRO:HD2	1.95	0.49
1:B:156:HIS:CD2	1:B:310:SER:HB3	2.48	0.49
1:B:333:VAL:HG22	1:B:389:ALA:HB2	1.94	0.49
1:C:83:ALA:CB	1:C:168:ILE:HA	2.43	0.49
1:C:149:ASP:CG	1:C:152:GLY:H	2.20	0.49
1:C:156:HIS:HA	1:C:311:THR:O	2.12	0.49
1:A:99:TRP:HA	1:A:102:THR:O	2.14	0.48
1:B:268:PRO:O	1:B:297:ARG:HB2	2.13	0.48
1:C:88:TRP:CZ3	1:C:287:SER:HA	2.49	0.48
1:A:16:LYS:HB2	1:A:56:GLY:H	1.77	0.48
1:B:11:SER:HB2	1:B:59:LYS:HB3	1.96	0.48
1:B:73:SER:O	1:B:74:TRP:CD1	2.67	0.48
1:B:192:SER:O	1:B:196:ILE:HG13	2.13	0.47
1:B:231:ILE:HG13	1:B:256:ILE:HG21	1.96	0.47
1:A:142:THR:HG23	1:A:142:THR:O	2.14	0.47
1:C:168:ILE:O	1:C:169:GLY:C	2.56	0.47
1:C:312:TYR:HE1	1:C:320:LEU:HD21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:SER:HB3	1:C:324:ALA:HB1	1.96	0.47
1:A:80:THR:HB	3:A:556:HOH:O	2.13	0.47
1:C:143:LYS:O	1:C:146:ASP:HB2	2.14	0.47
1:A:230:VAL:HG22	1:A:334:VAL:HG22	1.97	0.47
1:C:208:ASP:C	1:C:210:VAL:H	2.22	0.47
1:B:93:VAL:HG22	1:B:387:VAL:HG23	1.96	0.47
1:C:312:TYR:CE1	1:C:320:LEU:HD21	2.49	0.47
1:C:333:VAL:HG21	1:C:387:VAL:HG23	1.97	0.47
1:B:6:ILE:HD11	1:B:62:PHE:CE2	2.51	0.46
1:C:186:ASP:C	1:C:186:ASP:OD1	2.59	0.46
1:B:23:LEU:HD21	3:B:407:HOH:O	2.15	0.46
1:A:152:GLY:HA2	1:A:313:PRO:CD	2.46	0.46
1:C:166:ASN:HB2	3:C:508:HOH:O	2.15	0.46
1:C:369:THR:O	1:C:388:ARG:HD3	2.15	0.46
1:B:11:SER:OG	3:B:597:HOH:O	2.21	0.46
1:B:303:ALA:HB1	1:B:304:PRO:CD	2.46	0.46
1:B:371:ASP:H	1:B:388:ARG:HD2	1.80	0.46
1:B:82:PRO:HG2	1:B:83:ALA:H	1.80	0.45
1:A:95:ALA:N	1:A:96:PRO:CD	2.79	0.45
1:C:156:HIS:CD2	1:C:310:SER:HB3	2.52	0.45
1:C:222:ASP:HB3	1:C:225:ASP:HB2	1.98	0.45
1:B:89:GLY:HA2	1:B:304:PRO:HG2	1.97	0.45
1:C:119:ASP:OD1	1:C:314:ASP:N	2.42	0.45
1:C:25:ILE:HD13	1:C:54:MET:HE1	1.97	0.45
1:B:218:ILE:HD11	3:B:450:HOH:O	2.17	0.45
1:C:245:TYR:CE1	1:C:249:ILE:HD11	2.52	0.45
1:C:286:ASP:CA	1:C:306:VAL:HG13	2.47	0.45
1:B:193:TYR:CD1	1:B:241:ASP:OD2	2.69	0.45
1:C:122:HIS:O	1:C:126:ALA:HB2	2.17	0.45
1:A:333:VAL:HG21	1:A:387:VAL:CG1	2.47	0.45
1:B:29:ILE:HG23	1:B:39:VAL:HG21	1.98	0.45
1:B:64:HIS:HD2	1:B:241:ASP:OD2	2.00	0.44
1:B:156:HIS:CG	1:B:310:SER:HB3	2.52	0.44
1:C:274:ALA:O	3:C:407:HOH:O	2.21	0.44
1:B:89:GLY:CA	1:B:304:PRO:HG2	2.47	0.44
1:A:338:GLN:HE21	1:A:338:GLN:CA	2.28	0.44
1:B:111:VAL:HB	1:B:179:ILE:HD13	1.99	0.44
1:B:220:ALA:HB3	1:B:254:ALA:O	2.17	0.44
1:C:308:ILE:HG13	1:C:325:MET:HB3	1.99	0.44
1:C:208:ASP:C	1:C:210:VAL:N	2.75	0.44
1:A:338:GLN:HA	1:A:338:GLN:NE2	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:GLU:OE2	1:B:367:HIS:CE1	2.64	0.43
1:C:73:SER:O	1:C:74:TRP:C	2.61	0.43
1:B:193:TYR:HD1	1:B:241:ASP:OD2	2.01	0.43
1:C:34:LYS:H	1:C:34:LYS:HG3	1.70	0.43
1:C:71:LYS:HA	1:C:71:LYS:HD3	1.82	0.43
1:B:14:LYS:HA	1:B:14:LYS:HD3	1.78	0.43
1:B:11:SER:HB2	1:B:59:LYS:HB2	1.99	0.43
1:B:321:MET:C	1:B:325:MET:HE3	2.41	0.43
1:C:17:PHE:O	1:C:19:PRO:HD3	2.17	0.43
1:A:240:ASP:OD2	1:A:240:ASP:C	2.60	0.43
1:B:206:GLY:HA3	1:B:207:PRO:HD3	1.87	0.43
1:B:228:ALA:O	1:B:256:ILE:HG12	2.19	0.43
1:C:88:TRP:CH2	1:C:287:SER:HA	2.54	0.43
1:A:277:PRO:HG2	1:A:278:GLU:OE1	2.18	0.43
1:B:14:LYS:HE3	3:B:516:HOH:O	2.18	0.43
1:B:6:ILE:HD11	1:B:62:PHE:CD2	2.54	0.43
1:A:204:ILE:HG12	1:A:256:ILE:HD12	2.01	0.43
1:A:198:ILE:O	1:A:201:GLU:HB3	2.19	0.43
1:C:185:LEU:HD23	1:C:191:GLY:HA3	2.00	0.42
1:A:222:ASP:HA	1:A:223:PRO:HD2	1.71	0.42
1:C:327:THR:HB	1:C:328:PRO:CD	2.50	0.42
1:A:52:LYS:HG3	1:C:74:TRP:CD1	2.54	0.42
1:C:235:LEU:HD23	1:C:235:LEU:C	2.45	0.42
1:C:338:GLN:HA	1:C:338:GLN:NE2	2.27	0.42
1:B:120:TYR:HE1	1:B:148:ALA:HB2	1.85	0.42
1:C:83:ALA:HB3	1:C:167:ASP:O	2.19	0.42
1:C:149:ASP:OD1	1:C:152:GLY:CA	2.68	0.42
1:B:9:ILE:HD12	1:B:9:ILE:N	2.34	0.42
1:B:73:SER:HB2	1:B:319:THR:HG22	2.02	0.42
1:B:213:LYS:HE3	3:B:619:HOH:O	2.19	0.42
1:C:18:ASN:OD1	1:C:20:HIS:HB2	2.19	0.42
1:C:116:THR:O	1:C:183:ARG:HD2	2.20	0.42
1:B:118:VAL:O	1:B:118:VAL:HG13	2.19	0.42
1:A:234:SER:HB3	1:A:324:ALA:HB1	2.02	0.42
1:B:313:PRO:HA	1:B:314:ASP:HA	1.74	0.42
1:C:352:GLY:CA	1:C:363:ARG:HB2	2.49	0.42
1:C:352:GLY:HA2	1:C:361:THR:HG23	2.01	0.42
1:A:86:ILE:HB	1:B:5:THR:HG22	2.02	0.41
1:B:294:PHE:CE1	1:B:322:GLY:HA2	2.55	0.41
1:C:68:LEU:HD13	1:C:189:GLY:HA3	2.01	0.41
1:C:131:TRP:CE2	1:C:207:PRO:HD3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:TRP:HB3	1:C:180:TYR:CD1	2.55	0.41
1:C:74:TRP:C	1:C:74:TRP:CD1	2.98	0.41
1:C:355:ASP:HB2	3:C:556:HOH:O	2.20	0.41
1:B:136:LEU:HD11	1:B:183:ARG:CZ	2.50	0.41
1:A:10:VAL:HG12	1:A:12:VAL:HG12	2.00	0.41
1:A:318:GLU:CG	1:C:46:ASN:CG	2.93	0.41
1:C:322:GLY:N	1:C:325:MET:HE2	2.35	0.41
1:B:269:SER:HB3	1:B:298:GLN:NE2	2.35	0.41
1:A:344:LYS:HE3	3:A:650:HOH:O	2.20	0.41
1:B:377:GLY:O	1:B:378:TRP:C	2.63	0.41
1:A:213:LYS:HG3	1:A:214:ASP:HB3	2.03	0.41
1:A:265:GLU:N	1:A:296:ASN:HD21	2.14	0.41
1:A:369:THR:HB	1:A:391:LEU:HD13	2.03	0.41
1:B:234:SER:HB3	1:B:324:ALA:HB1	2.02	0.41
1:C:84:GLN:HB2	1:C:168:ILE:O	2.21	0.41
1:A:230:VAL:CG2	1:A:334:VAL:HG22	2.50	0.41
1:C:25:ILE:HD13	1:C:54:MET:CE	2.50	0.41
1:C:330:VAL:O	1:C:334:VAL:HG13	2.21	0.41
1:C:298:GLN:N	1:C:299:PRO:HD3	2.36	0.40
1:C:327:THR:N	1:C:328:PRO:HD2	2.35	0.40
1:C:139:LYS:HG3	1:C:139:LYS:O	2.21	0.40
1:C:114:LEU:N	1:C:114:LEU:CD1	2.84	0.40
1:C:286:ASP:HB3	1:C:306:VAL:HG13	2.03	0.40
1:B:200:ILE:HG23	1:B:231:ILE:HD13	2.03	0.40
1:A:48:VAL:HG12	1:C:74:TRP:HB3	2.03	0.40
1:B:351:VAL:O	1:B:352:GLY:C	2.65	0.40
1:C:73:SER:HB2	1:C:319:THR:HG22	2.04	0.40
1:C:342:TYR:O	1:C:345:TYR:O	2.39	0.40

All (2) 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)
3:A:518:HOH:O	3:C:649:HOH:O[2_565]	1.53	0.67
3:B:634:HOH:O	3:C:555:HOH:O[1_556]	1.84	0.36

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	393/398 (99%)	364 (93%)	26 (7%)	3 (1%)	16	8
1	B	389/398 (98%)	356 (92%)	27 (7%)	6 (2%)	8	2
1	C	385/398 (97%)	354 (92%)	26 (7%)	5 (1%)	9	3
All	All	1167/1194 (98%)	1074 (92%)	79 (7%)	14 (1%)	10	4

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	GLY
1	B	51	LEU
1	B	206	GLY
1	C	119	ASP
1	C	169	GLY
1	C	206	GLY
1	A	105	SER
1	B	22	VAL
1	B	352	GLY
1	A	167	ASP
1	B	271	SER
1	C	208	ASP
1	C	372	ASP
1	B	82	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	304/306 (99%)	273 (90%)	31 (10%)	7	2
1	B	305/306 (100%)	270 (88%)	35 (12%)	5	1
1	C	301/306 (98%)	258 (86%)	43 (14%)	3	1
All	All	910/918 (99%)	801 (88%)	109 (12%)	5	1

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	6	ILE
1	A	8	VAL
1	A	14	LYS
1	A	22	VAL
1	A	23	LEU
1	A	34	LYS
1	A	39	VAL
1	A	46	ASN
1	A	51	LEU
1	A	52	LYS
1	A	53	LYS
1	A	68	LEU
1	A	73	SER
1	A	80	THR
1	A	93	VAL
1	A	106	VAL
1	A	133	VAL
1	A	139	LYS
1	A	142	THR
1	A	145	ARG
1	A	183	ARG
1	A	213	LYS
1	A	248	ILE
1	A	297	ARG
1	A	318	GLU
1	A	334	VAL
1	A	338	GLN
1	A	387	VAL
1	A	388	ARG
1	A	391	LEU
1	B	2	GLU
1	B	4	ASN
1	B	5	THR

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Mol	Chain	Res	Type
1	B	6	ILE
1	B	8	VAL
1	B	14	LYS
1	B	21	GLU
1	B	39	VAL
1	B	41	VAL
1	B	53	LYS
1	B	59	LYS
1	B	67	VAL
1	B	71	LYS
1	B	73	SER
1	B	80	THR
1	B	91	GLU
1	B	93	VAL
1	B	133	VAL
1	B	177	VAL
1	B	183	ARG
1	B	213	LYS
1	B	235	LEU
1	B	248	ILE
1	B	295	SER
1	B	297	ARG
1	B	315	ASP
1	B	334	VAL
1	B	338	GLN
1	B	358	SER
1	B	359	LYS
1	B	361	THR
1	B	368	ILE
1	B	388	ARG
1	B	391	LEU
1	B	394	GLN
1	C	5	THR
1	C	6	ILE
1	C	8	VAL
1	C	9	ILE
1	C	10	VAL
1	C	20	HIS
1	C	22	VAL
1	C	23	LEU
1	C	29	ILE
1	C	32	GLN

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Mol	Chain	Res	Type
1	C	39	VAL
1	C	48	VAL
1	C	51	LEU
1	C	59	LYS
1	C	65	GLN
1	C	68	LEU
1	C	73	SER
1	C	81	GLN
1	C	93	VAL
1	C	96	PRO
1	C	106	VAL
1	C	133	VAL
1	C	141	SER
1	C	142	THR
1	C	143	LYS
1	C	144	LEU
1	C	145	ARG
1	C	147	CYS
1	C	177	VAL
1	C	188	ARG
1	C	235	LEU
1	C	242	SER
1	C	271	SER
1	C	297	ARG
1	C	306	VAL
1	C	334	VAL
1	C	338	GLN
1	C	356	ASP
1	C	359	LYS
1	C	361	THR
1	C	365	ILE
1	C	386	VAL
1	C	388	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	122	HIS
1	A	150	GLN
1	A	290	ASN
1	A	296	ASN

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Mol	Chain	Res	Type
1	A	338	GLN
1	A	367	HIS
1	B	4	ASN
1	B	18	ASN
1	B	64	HIS
1	B	65	GLN
1	B	81	GLN
1	B	122	HIS
1	B	202	GLN
1	B	296	ASN
1	B	338	GLN
1	B	367	HIS
1	B	394	GLN
1	C	28	HIS
1	C	64	HIS
1	C	122	HIS
1	C	150	GLN
1	C	296	ASN
1	C	298	GLN
1	C	329	HIS
1	C	338	GLN
1	C	360	ASN
1	C	367	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	395/398 (99%)	-0.39	0 100 100	18, 32, 53, 67	0
1	B	393/398 (98%)	-0.23	2 (0%) 87 89	24, 35, 52, 81	0
1	C	389/398 (97%)	-0.17	5 (1%) 75 77	19, 35, 57, 80	0
All	All	1177/1194 (98%)	-0.26	7 (0%) 85 88	18, 34, 54, 81	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	144	LEU	3.2
1	B	74	TRP	2.6
1	C	83	ALA	2.3
1	C	211	ALA	2.2
1	B	398	GLY	2.2
1	C	315	ASP	2.1
1	C	142	THR	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	A	401	1/1	0.96	0.05	60,60,60,60	0
2	CA	B	399	1/1	0.98	0.03	44,44,44,44	0
2	CA	B	402	1/1	0.98	0.04	47,47,47,47	0
2	CA	B	403	1/1	0.98	0.03	35,35,35,35	0
2	CA	C	399	1/1	0.98	0.03	44,44,44,44	0
2	CA	A	400	1/1	0.99	0.04	52,52,52,52	0
2	CA	B	400	1/1	0.99	0.03	34,34,34,34	0
2	CA	B	401	1/1	0.99	0.04	28,28,28,28	0
2	CA	A	399	1/1	0.99	0.02	24,24,24,24	0
2	CA	A	402	1/1	0.99	0.02	36,36,36,36	0
2	CA	A	403	1/1	0.99	0.03	37,37,37,37	0
2	CA	C	400	1/1	0.99	0.03	39,39,39,39	0
2	CA	C	401	1/1	0.99	0.03	26,26,26,26	0
2	CA	C	402	1/1	0.99	0.02	39,39,39,39	0
2	CA	C	403	1/1	0.99	0.03	36,36,36,36	0
2	CA	A	404	1/1	1.00	0.02	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.