W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:12 AM GMT

PDB ID	:	2ZWO
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)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	Percentile Ranks	Value
Rfree		0.191
Clashscore		16
Ramachandran outliers		1.2%
Sidechain outliers		9.9%
RSRZ outliers		1.7%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
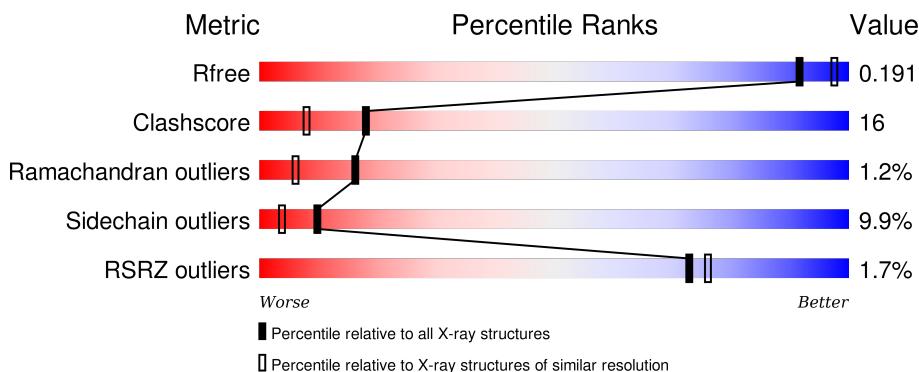
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	1799 (2.08-2.04)
Clashscore	102246	1910 (2.08-2.04)
Ramachandran outliers	100387	1893 (2.08-2.04)
Sidechain outliers	100360	1893 (2.08-2.04)
RSRZ outliers	91569	1802 (2.08-2.04)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	2% 73% 22% · ··
1	B	398	3% 66% 26% 6% ··
1	C	398	% 62% 29% 6% ··
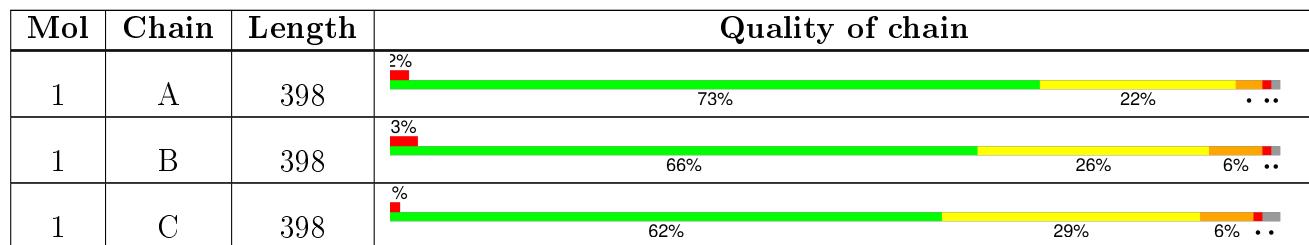
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CA	B	403	-	-	-	X

2 Entry composition (i)

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 2890	C 1830	N 484	O 569	S 7	0	0	0
1	B	393	Total 2888	C 1828	N 483	O 570	S 7	0	0	0
1	C	389	Total 2857	C 1811	N 478	O 561	S 7	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is water.

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

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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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

Chain A:

- Molecule 1: Tk-subtilisin

Chain B:

- Molecule 1: Tk-subtilisin

Chain C:
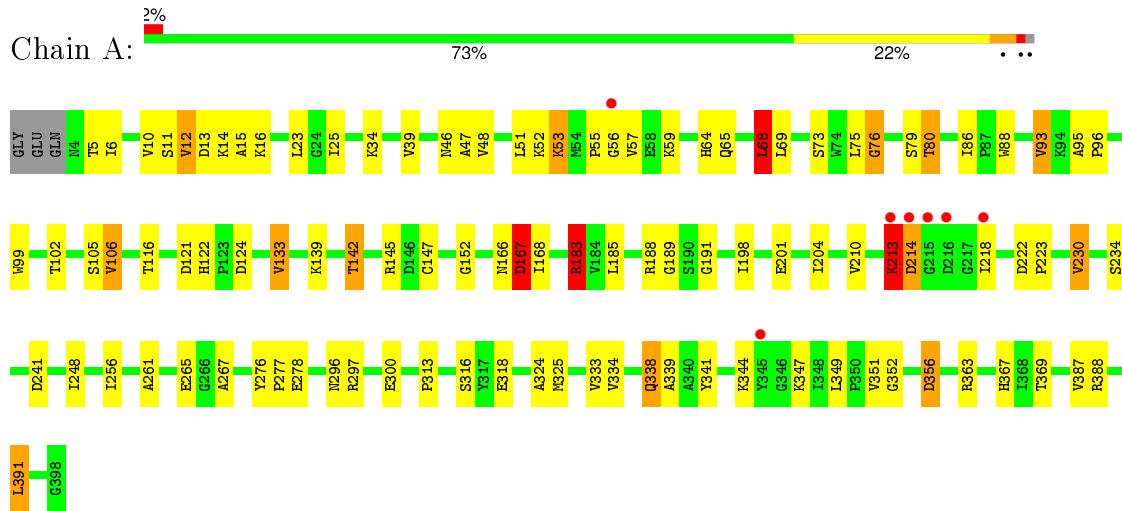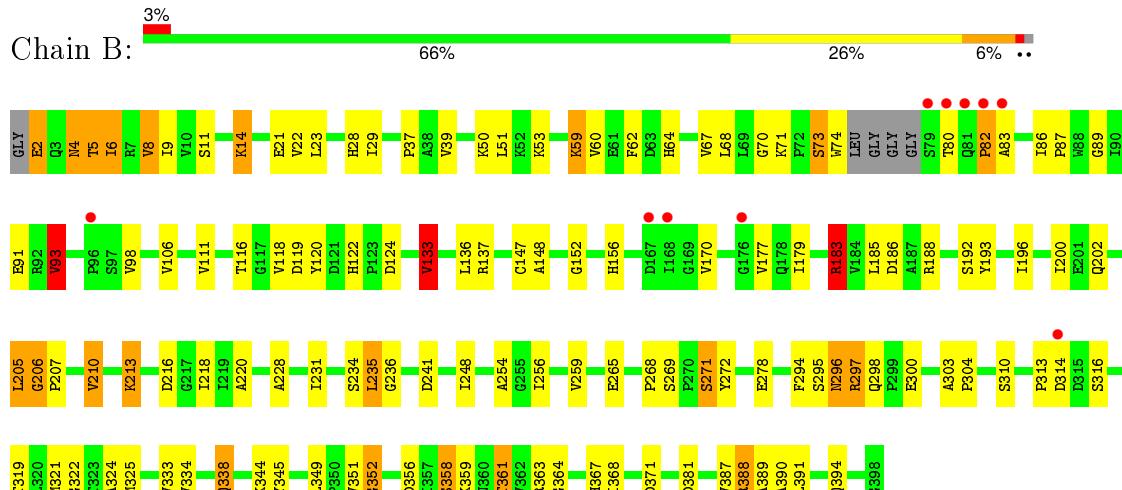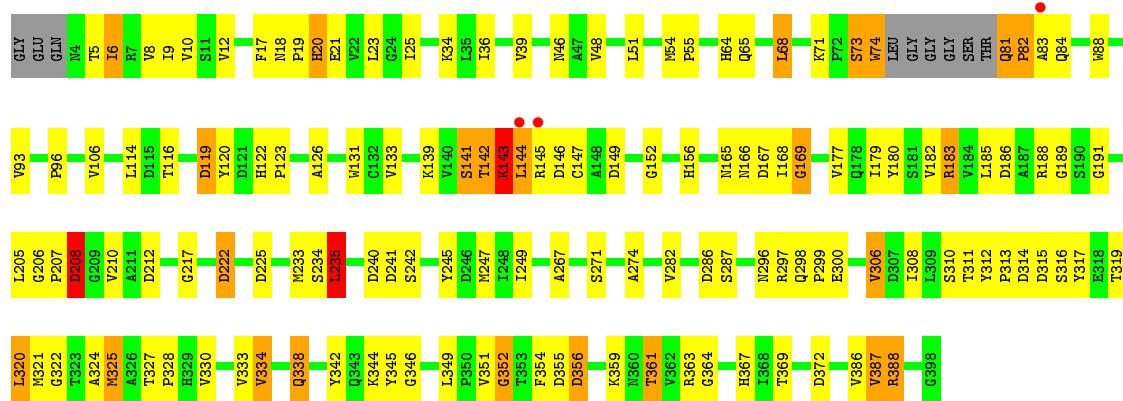
4 Data and refinement statistics (i)

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 46.86 – 2.07	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.63-2.07) 96.3 (46.86-2.07)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.08 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.184 , 0.227 0.185 , 0.191	Depositor DCC
R_{free} test set	3973 reflections (5.27%)	DCC
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 , 57.6	EDS
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
L-test for twinning [2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Outliers	2 of 79345 reflections (0.003%)	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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	1.02	1/2951 (0.0%)	1.01	8/4038 (0.2%)
1	B	0.95	1/2948 (0.0%)	1.01	16/4033 (0.4%)
1	C	1.00	1/2917 (0.0%)	1.05	13/3991 (0.3%)
All	All	0.99	3/8816 (0.0%)	1.03	37/12062 (0.3%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	282	VAL	CB-CG2	6.92	1.67	1.52
1	A	230	VAL	CB-CG2	5.47	1.64	1.52
1	B	210	VAL	C-O	5.35	1.33	1.23

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	183	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	A	183	ARG	NE-CZ-NH2	-10.38	115.11	120.30
1	C	183	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	C	351	VAL	C-N-CA	-8.06	105.38	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	183	ARG	NE-CZ-NH2	-8.03	116.29	120.30
1	A	93	VAL	CG1-CB-CG2	7.70	123.22	110.90
1	C	387	VAL	CG1-CB-CG2	7.54	122.97	110.90
1	B	235	LEU	CA-CB-CG	7.01	131.42	115.30
1	B	381	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	C	320	LEU	CA-CB-CG	6.89	131.16	115.30
1	C	325	MET	CG-SD-CE	-6.84	89.26	100.20
1	B	93	VAL	CG1-CB-CG2	6.62	121.49	110.90
1	B	216	ASP	CB-CG-OD1	-6.51	112.44	118.30
1	B	235	LEU	CB-CG-CD2	6.42	121.91	111.00
1	B	137	ARG	NE-CZ-NH1	-6.41	117.09	120.30
1	B	183	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	C	142	THR	N-CA-C	-6.18	94.31	111.00
1	B	388	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	C	235	LEU	CA-CB-CG	6.10	129.33	115.30
1	B	119	ASP	CB-CG-OD2	6.02	123.72	118.30
1	C	320	LEU	CB-CG-CD2	5.86	120.96	111.00
1	C	240	ASP	CB-CG-OD2	5.83	123.55	118.30
1	B	119	ASP	CB-CG-OD1	-5.75	113.13	118.30
1	B	183	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	68	LEU	CB-CG-CD1	-5.64	101.41	111.00
1	C	222	ASP	CB-CG-OD2	5.46	123.21	118.30
1	C	208	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	93	VAL	CA-CB-CG1	5.26	118.79	110.90
1	B	185	LEU	CB-CG-CD2	5.26	119.94	111.00
1	B	133	VAL	CB-CA-C	-5.22	101.47	111.40
1	B	186	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	351	VAL	C-N-CA	-5.22	111.35	122.30
1	B	188	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	B	351	VAL	C-N-CA	-5.19	111.41	122.30
1	A	183	ARG	CD-NE-CZ	5.14	130.80	123.60
1	A	133	VAL	CB-CA-C	-5.10	101.71	111.40
1	C	6	ILE	CG1-CB-CG2	5.08	122.59	111.40

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	Mainchain,Peptide
1	A	12	VAL	Peptide
1	A	166	ASN	Mainchain
1	A	167	ASP	Mainchain,Peptide
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	Mainchain,Peptide
1	B	259	VAL	Mainchain
1	B	271	SER	Mainchain
1	B	4	ASN	Mainchain
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	Mainchain,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	2890	0	2851	67	0
1	B	2888	0	2844	106	0
1	C	2857	0	2818	103	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	251	0	0	12	1
3	C	220	0	0	3	2
All	All	9389	0	8513	269	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 (269) 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:338:GLN:HA	1:B:338:GLN:HE21	1.05	1.10
1:C:361:THR:HG22	1:C:364:GLY:H	1.21	1.03
1:B:352:GLY:HA3	1:B:363:ARG:HB2	1.41	0.98
1:C:321:MET:C	1:C:325:MET:CE	2.33	0.96
1:B:321:MET:C	1:B:325:MET:HE2	1.89	0.93
1:A:352:GLY:HA3	1:A:363:ARG:HB2	1.51	0.91
1:C:321:MET:O	1:C:325:MET:HE3	1.71	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:338:GLN:HA	1:B:338:GLN:NE2	1.87	0.88
1:B:344:LYS:HE2	1:B:345:TYR:OH	1.75	0.85
1:C:321:MET:C	1:C:325:MET:HE3	1.94	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:CA	1:B:338:GLN:HE21	1.89	0.79
1:B:356:ASP:OD1	1:B:361:THR:HG21	1.83	0.79
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:MET:C	1:B:325:MET:CE	2.56	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:C:321:MET:O	1:C:325:MET:CE	2.38	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: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
1:A:52:LYS:HD3	1:A:52:LYS:O	1.93	0.68
1:B:70:GLY:CA	1:B:325:MET:CE	2.72	0.68
1:B:70:GLY:HA3	1:B:325:MET:HE3	1.75	0.68
1:C:352:GLY:HA3	1:C:361:THR:HG23	1.76	0.67
1:A:265:GLU:H	1:A:296:ASN:HD21	1.42	0.67
1:B:70:GLY:CA	1:B:325:MET:HE3	2.26	0.66
1:B:70:GLY:HA3	1:B:325:MET:CE	2.25	0.66
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:321:MET:C	1:C:325:MET:HE2	2.15	0.66
1:B:70:GLY:HA2	1:B:325:MET:HE1	1.76	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:6:ILE:HD11	1:C:48:VAL:CG2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:70:GLY:HA2	1:B:325:MET:CE	2.33	0.58
1:A:25:ILE:HD13	1:A:47:ALA:HB1	1.83	0.58
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:B:152:GLY:HA2	1:B:313:PRO:CD	2.36	0.56
1:B:321:MET:CA	1:B:325:MET:HE2	2.35	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
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:HD12	1:C:9:ILE:N	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:C:119:ASP:HB2	1:C:313:PRO:HB3	1.89	0.54
1:A:369:THR:O	1:A:388:ARG:HD3	2.08	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: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:B:394:GLN:NE2	1:B:394:GLN:HA	2.23	0.54
1:B:202:GLN:O	1:B:206:GLY:HA2	2.08	0.53
1:A:13:ASP:OD1	1:A:15:ALA:HB3	2.08	0.53
1:B:11:SER:HB2	1:B:59:LYS:CB	2.39	0.53
1:C:352:GLY:HA3	1:C:361:THR:CG2	2.39	0.53
1:C:212:ASP:OD2	1:C:217:GLY:N	2.37	0.53
1:B:278:GLU:N	1:B:278:GLU:OE1	2.41	0.53
1:C:352:GLY:CA	1:C:361:THR:CG2	2.87	0.52
1:C:114:LEU:HA	1:C:182:VAL:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:HIS:HB3	3:B:484:HOH:O	2.08	0.52
1:B:265:GLU:H	1:B:296:ASN:ND2	2.04	0.52
1:B:296:ASN:HD22	1:B:296:ASN:N	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:C:73:SER:CB	1:C:319:THR:HG22	2.40	0.51
1:B:170:VAL:HG21	1:B:310:SER:HA	1.92	0.51
1:B:356:ASP:O	1:B:367:HIS:CD2	2.63	0.51
1:A:300:GLU:OE2	1:A:367:HIS:CE1	2.62	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
1:B:205:LEU:O	1:B:210:VAL:O	2.29	0.51
1:B:344:LYS:CE	1:B:345:TYR:OH	2.55	0.51
1:A:338:GLN:HE22	1:A:349:LEU:HB2	1.75	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:B:14:LYS:HE2	1:B:37:PRO:HA	1.92	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:C:322:GLY:N	1:C:325:MET:CE	2.74	0.49
1:B:70:GLY:CA	1:B:325:MET:HE1	2.38	0.49
1:A:122:HIS:HE1	1:A:316:SER:O	1.95	0.49
1:A:318:GLU:HG2	1:C:46:ASN:CG	2.32	0.49
1:C:114:LEU:HD12	1:C:114:LEU:N	2.27	0.49
1:C:21:GLU:OE2	1:C:55:PRO:HD2	2.11	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:156:HIS:HA	1:C:311:THR:O	2.12	0.49
1:A:121:ASP:OD2	1:A:121:ASP:C	2.51	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:321:MET:N	1:B:325:MET:HE2	2.30	0.47
1:C:312:TYR:HE1	1:C:320:LEU:HD21	1.79	0.47
1:A:142:THR:O	1:A:142:THR:HG23	2.14	0.47
1:C:234:SER:HB3	1:C:324:ALA:HB1	1.96	0.47
1:C:314:ASP:O	1:C:315:ASP:C	2.52	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:312:TYR:CE1	1:C:320:LEU:HD21	2.49	0.47
1:B:93:VAL:HG22	1:B:387:VAL:HG23	1.96	0.47
1:C:333:VAL:HG21	1:C:387:VAL:HG23	1.97	0.47
1:B:356:ASP:CG	1:B:361:THR:HG21	2.35	0.46
1:B:6:ILE:HD11	1:B:62:PHE:CE2	2.51	0.46
1:C:322:GLY:N	1:C:325:MET:HE2	2.30	0.46
1:B:23:LEU:HD21	3:B:407:HOH:O	2.15	0.46
1:C:369:THR:O	1:C:388:ARG:HD3	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:354:PHE:CD2	1:C:354:PHE:C	2.89	0.46
1:B:371:ASP:H	1:B:388:ARG:HD2	1.80	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: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:149:ASP:CG	1:C:152:GLY:H	2.20	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:218:ILE:HD11	3:B:450:HOH:O	2.17	0.45
1:B:86:ILE:O	1:B:87:PRO:C	2.52	0.45
1:C:122:HIS:O	1:C:126:ALA:HB2	2.17	0.45
1:B:193:TYR:CD1	1:B:241:ASP:OD2	2.69	0.45
1:B:29:ILE:HG23	1:B:39:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:VAL:HG21	1:A:387:VAL:CG1	2.47	0.45
1:B:156:HIS:CG	1:B:310:SER:HB3	2.52	0.44
1:B:64:HIS:HD2	1:B:241:ASP:OD2	2.00	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:CA	1:A:338:GLN:HE21	2.28	0.44
1:B:111:VAL:HB	1:B:179:ILE:HD13	1.99	0.44
1:C:308:ILE:HG13	1:C:325:MET:HB3	1.99	0.44
1:B:220:ALA:HB3	1:B:254:ALA:O	2.17	0.44
1:B:300:GLU:OE2	1:B:367:HIS:CE1	2.64	0.43
1:A:338:GLN:NE2	1:A:338:GLN:HA	2.28	0.43
1:C:34:LYS:HG3	1:C:34:LYS:H	1.70	0.43
1:B:193:TYR:HD1	1:B:241:ASP:OD2	2.01	0.43
1:C:71:LYS:HD3	1:C:71:LYS:HA	1.82	0.43
1:B:14:LYS:HD3	1:B:14:LYS:HA	1.78	0.43
1:B:11:SER:HB2	1:B:59:LYS:HB2	1.99	0.43
1:C:36:ILE:HG12	1:C:247:MET:HE2	2.01	0.43
1:C:17:PHE:O	1:C:19:PRO:HD3	2.17	0.43
1:C:168:ILE:O	1:C:169:GLY:C	2.56	0.43
1:B:206:GLY:HA3	1:B:207:PRO:HD3	1.87	0.43
1:C:88:TRP:CH2	1:C:287:SER:HA	2.54	0.43
1:B:228:ALA:O	1:B:256:ILE:HG12	2.19	0.43
1:B:14:LYS:HE3	3:B:516:HOH:O	2.18	0.43
1:A:277:PRO:HG2	1:A:278:GLU:OE1	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:C:338:GLN:NE2	1:C:338:GLN:HA	2.27	0.42
1:A:52:LYS:HG3	1:C:74:TRP:CD1	2.54	0.42
1:C:208:ASP:C	1:C:210:VAL:H	2.22	0.42
1:C:83:ALA:HB3	1:C:167:ASP:O	2.19	0.42
1:B:120:TYR:HE1	1:B:148:ALA:HB2	1.85	0.42
1:C:149:ASP:OD1	1:C:152:GLY:CA	2.68	0.42
1:B:73:SER:HB2	1:B:319:THR:HG22	2.02	0.42
1:C:116:THR:O	1:C:183:ARG:HD2	2.20	0.42
1:B:9:ILE:N	1:B:9:ILE:HD12	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:VAL:O	1:B:118:VAL:HG13	2.19	0.42
1:C:352:GLY:HA2	1:C:361:THR:HG23	2.01	0.42
1:C:352:GLY:CA	1:C:363:ARG:HB2	2.49	0.42
1:B:313:PRO:HA	1:B:314:ASP:HA	1.74	0.42
1:A:234:SER:HB3	1:A:324:ALA:HB1	2.02	0.42
1:C:68:LEU:HD13	1:C:189:GLY:HA3	2.01	0.41
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:131:TRP:CE2	1:C:207:PRO:HD3	2.55	0.41
1:C:131:TRP:HB3	1:C:180:TYR:CD1	2.55	0.41
1:C:355:ASP:HB2	3:C:556:HOH:O	2.20	0.41
1:C:186:ASP:C	1:C:186:ASP:OD1	2.59	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: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: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:C:84:GLN:HB2	1:C:168:ILE:O	2.21	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: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:327:THR:N	1:C:328:PRO:HD2	2.35	0.40
1:C:298:GLN:N	1:C:299:PRO:HD3	2.36	0.40
1:C:139:LYS:O	1:C:139:LYS:HG3	2.21	0.40
1:C:114:LEU:CD1	1:C:114:LEU:N	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: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

Full wwPDB X-ray Structure Validation Report

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	393/398 (99%)	364 (93%)	26 (7%)	3 (1%)	24	12
1	B	389/398 (98%)	356 (92%)	27 (7%)	6 (2%)	13	4
1	C	385/398 (97%)	354 (92%)	26 (7%)	5 (1%)	15	5
All	All	1167/1194 (98%)	1074 (92%)	79 (7%)	14 (1%)	16	6

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 ⓘ

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%)	278 (91%)	26 (9%)	13	6
1	B	305/306 (100%)	276 (90%)	29 (10%)	11	4
1	C	301/306 (98%)	266 (88%)	35 (12%)	7	2
All	All	910/918 (99%)	820 (90%)	90 (10%)	10	4

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	6	ILE
1	A	14	LYS
1	A	23	LEU
1	A	34	LYS
1	A	39	VAL
1	A	46	ASN
1	A	51	LEU
1	A	53	LYS
1	A	68	LEU
1	A	73	SER
1	A	80	THR
1	A	93	VAL
1	A	133	VAL
1	A	139	LYS
1	A	142	THR
1	A	145	ARG
1	A	147	CYS
1	A	183	ARG
1	A	213	LYS
1	A	248	ILE
1	A	297	ARG
1	A	325	MET
1	A	338	GLN
1	A	356	ASP
1	A	391	LEU
1	B	2	GLU
1	B	5	THR
1	B	6	ILE
1	B	8	VAL
1	B	14	LYS
1	B	53	LYS
1	B	59	LYS
1	B	67	VAL

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Mol	Chain	Res	Type
1	B	68	LEU
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	147	CYS
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	296	ASN
1	B	297	ARG
1	B	334	VAL
1	B	338	GLN
1	B	358	SER
1	B	361	THR
1	B	391	LEU
1	C	5	THR
1	C	8	VAL
1	C	10	VAL
1	C	20	HIS
1	C	23	LEU
1	C	39	VAL
1	C	51	LEU
1	C	65	GLN
1	C	68	LEU
1	C	73	SER
1	C	74	TRP
1	C	81	GLN
1	C	93	VAL
1	C	96	PRO
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

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Mol	Chain	Res	Type
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	386	VAL
1	C	388	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	64	HIS
1	A	122	HIS
1	A	150	GLN
1	A	290	ASN
1	A	296	ASN
1	A	338	GLN
1	A	367	HIS
1	B	4	ASN
1	B	64	HIS
1	B	65	GLN
1	B	122	HIS
1	B	150	GLN
1	B	296	ASN
1	B	298	GLN
1	B	338	GLN
1	B	367	HIS
1	C	64	HIS
1	C	122	HIS
1	C	150	GLN
1	C	296	ASN
1	C	298	GLN
1	C	338	GLN
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 carbohydrates 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.31	7 (1%)	71 74	18, 32, 53, 67	0
1	B	393/398 (98%)	-0.17	10 (2%)	61 65	24, 35, 52, 81	0
1	C	389/398 (97%)	-0.47	3 (0%)	87 89	19, 35, 57, 80	0
All	All	1177/1194 (98%)	-0.32	20 (1%)	73 76	18, 34, 54, 81	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	80	THR	4.3
1	B	82	PRO	3.5
1	A	345	TYR	3.4
1	B	81	GLN	3.4
1	B	83	ALA	3.2
1	C	83	ALA	3.1
1	A	218	ILE	3.1
1	B	79	SER	2.6
1	C	144	LEU	2.5
1	B	96	PRO	2.4
1	A	56	GLY	2.4
1	B	167	ASP	2.3
1	A	213	LYS	2.2
1	B	314	ASP	2.1
1	C	145	ARG	2.1
1	B	168	ILE	2.1
1	A	216	ASP	2.1
1	A	214	ASP	2.0
1	A	215	GLY	2.0
1	B	176	GLY	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors($Å^2$)	Q<0.9
2	CA	B	403	1/1	0.98	0.10	3.02	35,35,35,35	0
2	CA	C	401	1/1	0.99	0.11	1.50	26,26,26,26	0
2	CA	B	400	1/1	0.98	0.10	0.50	34,34,34,34	0
2	CA	A	399	1/1	0.99	0.12	0.40	24,24,24,24	0
2	CA	A	404	1/1	0.99	0.07	-0.61	35,35,35,35	0
2	CA	C	400	1/1	0.99	0.07	-1.18	39,39,39,39	0
2	CA	C	403	1/1	0.97	0.07	-1.24	36,36,36,36	0
2	CA	C	399	1/1	0.98	0.05	-1.48	44,44,44,44	0
2	CA	B	401	1/1	0.98	0.07	-1.55	28,28,28,28	0
2	CA	A	402	1/1	0.99	0.04	-1.98	36,36,36,36	0
2	CA	A	400	1/1	0.99	0.06	-2.58	52,52,52,52	0
2	CA	B	402	1/1	0.99	0.06	-2.78	47,47,47,47	0
2	CA	C	402	1/1	0.99	0.05	-2.79	39,39,39,39	0
2	CA	B	399	1/1	0.97	0.03	-3.60	44,44,44,44	0
2	CA	A	401	1/1	0.98	0.05	-	60,60,60,60	0
2	CA	A	403	1/1	0.99	0.07	-	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.