Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:11 AM GMT

PDB ID	:	2ZWP
Title	:	Crystal structure of Ca3 site mutant of Pro-S324A
Authors	:	Takeuchi, Y.; Tanaka, S.; Matsumura, H.; Koga, Y.; Takano, K.; Kanaya, S.
Deposited on	:	2008-12-17
Resolution	:	2.40 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

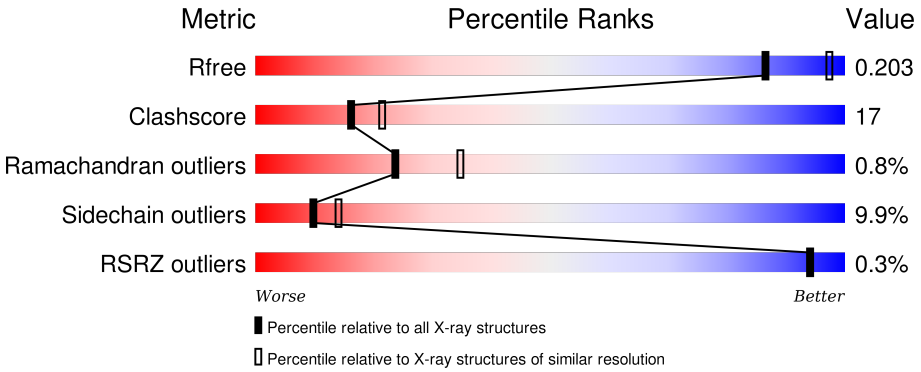
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	67% 26%
1	B	398	70% 21% 5%

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	A	400	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6103 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	389	Total	C	N	O	S	0	0	0
			2853	1811	476	559	7			
1	B	383	Total	C	N	O	S	0	0	0
			2821	1790	471	553	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	ALA	ASP	ENGINEERED	UNP P58502
A	324	ALA	SER	ENGINEERED	UNP P58502
B	225	ALA	ASP	ENGINEERED	UNP P58502
B	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	Ca	0	0
			5	5		
2	A	6	Total	Ca	0	0
			6	6		

- Molecule 3 is water.

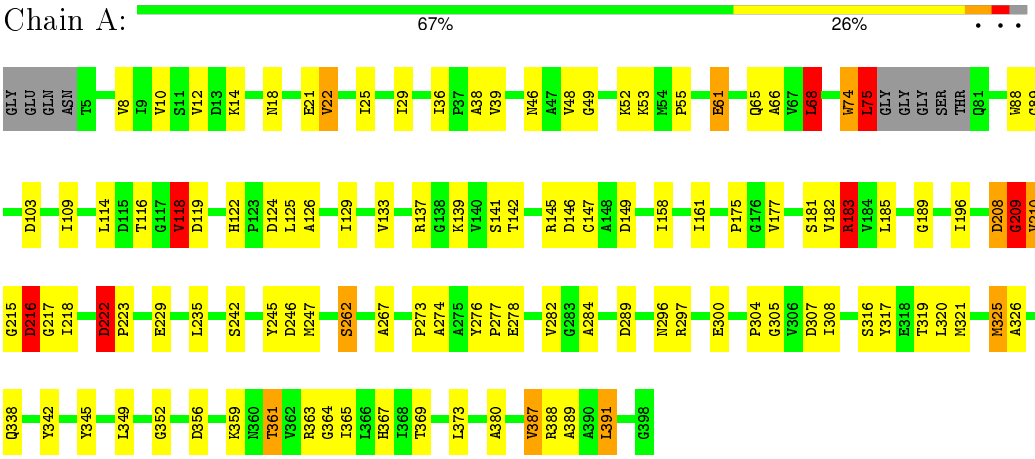
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	218	Total	O	0	0
			218	218		
3	B	200	Total	O	0	0
			200	200		

3 Residue-property plots (i)

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.

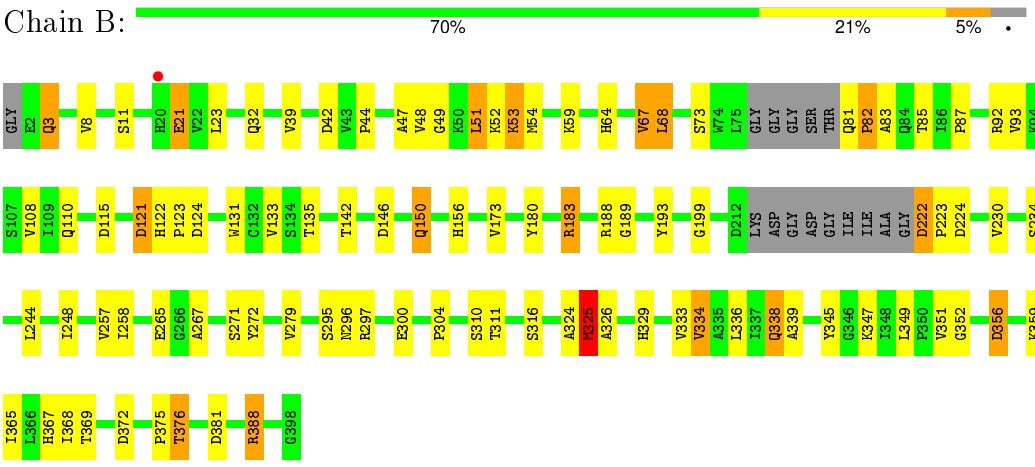
- Molecule 1: Tk-subtilisin

Chain A:



- Molecule 1: Tk-subtilisin

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	50.58Å 87.74Å 155.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.85 – 2.40 43.87 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.3 (43.85-2.40) 94.3 (43.87-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.80 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.157 , 0.202 0.157 , 0.203	Depositor DCC
R_{free} test set	1326 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	27.7	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 52.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 26269 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6103	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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	1.00	0/2913	1.01	12/3986 (0.3%)
1	B	0.98	1/2880 (0.0%)	0.99	12/3941 (0.3%)
All	All	0.99	1/5793 (0.0%)	1.00	24/7927 (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	1	5
1	B	0	2
All	All	1	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	193	TYR	CD2-CE2	5.26	1.47	1.39

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	75	LEU	CA-CB-CG	8.48	134.80	115.30
1	B	235	LEU	CA-CB-CG	6.80	130.95	115.30
1	A	118	VAL	CB-CA-C	-6.50	99.05	111.40
1	A	210	VAL	N-CA-C	-6.13	94.46	111.00
1	B	223	PRO	N-CA-C	6.07	127.87	112.10
1	A	183	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	213	LYS	N-CA-C	-5.95	94.94	111.00
1	A	209	GLY	N-CA-C	-5.87	98.44	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	325	MET	CG-SD-CE	5.76	109.42	100.20
1	B	222	ASP	CB-CA-C	5.62	121.63	110.40
1	A	222	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	42	ASP	CB-CG-OD1	5.45	123.21	118.30
1	A	118	VAL	CG1-CB-CG2	5.45	119.61	110.90
1	B	222	ASP	C-N-CD	-5.38	108.77	120.60
1	B	121	ASP	CB-CG-OD1	5.35	123.12	118.30
1	A	210	VAL	N-CA-CB	5.35	123.28	111.50
1	B	345	TYR	C-N-CA	-5.30	111.17	122.30
1	B	183	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	74	TRP	C-N-CA	5.20	134.70	121.70
1	B	51	LEU	CA-CB-CG	5.18	127.22	115.30
1	A	68	LEU	CA-CB-CG	5.15	127.14	115.30
1	A	149	ASP	CB-CG-OD2	5.05	122.84	118.30
1	B	67	VAL	CB-CA-C	5.04	120.97	111.40
1	B	8	VAL	CB-CA-C	5.03	120.95	111.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	216	ASP	CA

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	208	ASP	Peptide
1	A	209	GLY	Peptide
1	A	212	ASP	Peptide
1	A	213	LYS	Peptide
1	A	222	ASP	Peptide
1	B	222	ASP	Peptide
1	B	81	GLN	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	2853	0	2817	112	0
1	B	2821	0	2779	78	0
2	A	6	0	0	0	0
2	B	5	0	0	0	0
3	A	218	0	0	1	0
3	B	200	0	0	12	0
All	All	6103	0	5596	190	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (190) 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:361:THR:HG21	3:B:562:HOH:O	1.54	1.07
1:A:215:GLY:CA	1:A:216:ASP:HB3	1.86	1.04
1:B:361:THR:HG22	1:B:364:GLY:H	1.24	1.02
1:A:361:THR:HG22	1:A:364:GLY:H	1.23	1.02
1:A:215:GLY:HA3	1:A:216:ASP:CB	1.88	1.01
1:A:215:GLY:HA3	1:A:216:ASP:HB3	0.95	0.94
1:A:320:LEU:CB	1:A:325:MET:CE	2.48	0.92
1:A:122:HIS:HD2	1:A:124:ASP:H	1.18	0.90
1:B:359:LYS:HE3	1:B:368:ILE:HD11	1.56	0.87
1:A:320:LEU:HB3	1:A:325:MET:CE	2.04	0.87
1:A:213:LYS:H	1:A:214:ASP:HB3	1.39	0.86
1:B:3:GLN:HG2	1:B:44:PRO:HB3	1.57	0.86
1:B:64:HIS:HD2	1:B:241:ASP:OD2	1.60	0.84
1:A:320:LEU:HB2	1:A:325:MET:CE	2.08	0.83
1:A:212:ASP:OD1	1:A:213:LYS:NZ	2.09	0.83
1:B:234:SER:HB3	1:B:324:ALA:HB1	1.61	0.83
1:A:68:LEU:HD13	1:A:189:GLY:HA3	1.59	0.82
1:A:320:LEU:CB	1:A:325:MET:HE2	2.08	0.82
1:B:338:GLN:HA	1:B:338:GLN:HE21	1.44	0.81
1:A:356:ASP:OD2	1:A:361:THR:HG21	1.82	0.79
1:A:212:ASP:OD1	1:A:213:LYS:CE	2.30	0.79
1:A:320:LEU:CB	1:A:325:MET:HE3	2.13	0.78
1:B:361:THR:O	1:B:365:ILE:HD12	1.84	0.77
1:B:122:HIS:HD2	1:B:124:ASP:H	1.31	0.77
1:A:213:LYS:N	1:A:214:ASP:HB3	2.02	0.75
1:A:320:LEU:HB2	1:A:325:MET:HE2	1.64	0.74
1:B:300:GLU:OE2	1:B:367:HIS:HE1	1.73	0.72
1:A:214:ASP:OD1	1:A:215:GLY:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:VAL:O	1:A:337:ILE:HG13	1.93	0.69
1:A:88:TRP:CH2	1:A:304:PRO:HB3	2.29	0.68
1:A:212:ASP:OD1	1:A:213:LYS:HE3	1.93	0.68
1:A:126:ALA:HA	1:A:129:ILE:HD12	1.73	0.68
1:A:213:LYS:H	1:A:214:ASP:CB	2.05	0.68
1:A:212:ASP:HA	1:A:213:LYS:HE3	1.76	0.68
1:A:18:ASN:O	1:A:21:GLU:HG3	1.92	0.68
1:B:224:ASP:HB2	3:B:501:HOH:O	1.93	0.67
1:B:361:THR:CG2	1:B:364:GLY:H	2.03	0.66
1:A:137:ARG:HH21	1:A:139:LYS:NZ	1.93	0.66
1:B:279:VAL:O	3:B:561:HOH:O	2.12	0.66
1:A:213:LYS:NZ	1:A:216:ASP:OD2	2.30	0.65
1:A:213:LYS:HD2	1:A:214:ASP:HB3	1.79	0.65
1:A:75:LEU:HD22	1:A:307:ASP:CG	2.17	0.64
1:A:245:TYR:HE1	1:A:278:GLU:OE1	1.81	0.64
1:B:338:GLN:HA	1:B:338:GLN:NE2	2.12	0.64
1:A:213:LYS:HD2	1:A:214:ASP:CB	2.28	0.63
1:A:118:VAL:HG22	1:A:181:SER:OG	1.99	0.63
1:B:361:THR:HG22	1:B:364:GLY:N	2.06	0.63
1:B:300:GLU:OE2	1:B:367:HIS:CE1	2.52	0.62
1:B:369:THR:O	1:B:388:ARG:NH1	2.30	0.62
1:A:267:ALA:H	1:A:296:ASN:ND2	1.98	0.62
1:B:359:LYS:HE3	1:B:368:ILE:CD1	2.28	0.62
1:B:356:ASP:O	1:B:367:HIS:HD2	1.83	0.61
1:A:338:GLN:HE22	1:A:349:LEU:H	1.46	0.61
1:A:213:LYS:HB2	1:A:214:ASP:CB	2.31	0.61
1:B:95:ALA:N	1:B:96:PRO:CD	2.64	0.61
1:A:74:TRP:CB	1:A:75:LEU:HD13	2.31	0.60
1:B:106:VAL:HG12	1:B:339:ALA:HB1	1.83	0.60
1:B:356:ASP:CG	3:B:562:HOH:O	2.40	0.60
1:B:356:ASP:OD1	3:B:562:HOH:O	2.17	0.60
1:A:74:TRP:HB3	1:A:75:LEU:HD13	1.84	0.60
1:B:64:HIS:CD2	1:B:241:ASP:OD2	2.50	0.60
1:A:22:VAL:O	1:A:25:ILE:HG13	2.02	0.59
1:A:61:GLU:OE1	1:A:242:SER:HB2	2.02	0.59
1:A:320:LEU:HB3	1:A:325:MET:HE3	1.75	0.59
1:B:295:SER:O	1:B:297:ARG:NH1	2.35	0.59
1:B:234:SER:HB3	1:B:324:ALA:CB	2.32	0.59
1:B:304:PRO:O	1:B:326:ALA:HA	2.03	0.59
1:B:110:GLN:HG2	1:B:180:TYR:CZ	2.37	0.59
1:B:95:ALA:H	1:B:96:PRO:HD3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:HIS:CD2	1:A:124:ASP:H	2.10	0.57
1:A:185:LEU:HD21	1:A:235:LEU:HD22	1.86	0.57
1:A:342:TYR:O	1:A:345:TYR:O	2.21	0.57
1:A:114:LEU:HD12	1:A:114:LEU:N	2.19	0.57
1:B:352:GLY:HA3	1:B:361:THR:HG23	1.87	0.56
1:B:32:GLN:HG2	1:B:39:VAL:HG23	1.86	0.56
1:A:29:ILE:HD12	1:A:39:VAL:HG21	1.87	0.56
1:B:372:ASP:OD2	1:B:376:THR:O	2.23	0.56
1:A:118:VAL:HG13	1:A:158:ILE:HD12	1.88	0.55
1:B:23:LEU:HD12	3:B:428:HOH:O	2.05	0.55
1:B:265:GLU:H	1:B:296:ASN:ND2	2.04	0.55
1:A:213:LYS:CB	1:A:214:ASP:HB3	2.36	0.55
1:B:267:ALA:H	1:B:296:ASN:ND2	2.05	0.55
1:A:213:LYS:H	1:A:214:ASP:CA	2.21	0.54
1:B:376:THR:HG21	3:B:578:HOH:O	2.06	0.54
1:A:103:ASP:HB2	1:A:175:PRO:HD2	1.89	0.54
1:A:333:VAL:HG21	1:A:387:VAL:HG13	1.89	0.54
1:A:320:LEU:HB2	1:A:325:MET:HE3	1.80	0.53
1:A:213:LYS:HB2	1:A:214:ASP:HB3	1.89	0.53
1:B:258:ILE:HG22	1:B:279:VAL:HG13	1.90	0.53
1:B:338:GLN:HE22	1:B:349:LEU:H	1.55	0.53
1:B:297:ARG:NE	1:B:381:ASP:OD1	2.41	0.53
1:A:289:ASP:HB3	1:A:373:LEU:HD13	1.92	0.52
1:A:137:ARG:HH21	1:A:139:LYS:HZ2	1.57	0.52
1:A:114:LEU:N	1:A:114:LEU:CD1	2.73	0.52
1:A:212:ASP:CA	1:A:213:LYS:HE3	2.40	0.51
1:A:214:ASP:OD1	1:A:215:GLY:CA	2.58	0.51
1:A:361:THR:O	1:A:365:ILE:HG13	2.11	0.51
1:A:304:PRO:O	1:A:326:ALA:HA	2.10	0.51
1:A:320:LEU:C	1:A:325:MET:HE2	2.31	0.51
1:A:212:ASP:HA	1:A:213:LYS:HG3	1.93	0.51
1:B:352:GLY:CA	3:B:562:HOH:O	2.58	0.50
1:A:214:ASP:OD1	1:A:214:ASP:C	2.49	0.50
1:A:300:GLU:OE2	1:A:367:HIS:HE1	1.95	0.50
1:B:265:GLU:H	1:B:296:ASN:HD21	1.59	0.50
1:B:49:GLY:O	1:B:53:LYS:HE3	2.12	0.50
1:A:214:ASP:OD1	1:A:215:GLY:HA3	2.11	0.49
1:A:213:LYS:HB2	1:A:214:ASP:HB2	1.93	0.49
1:B:95:ALA:N	1:B:96:PRO:HD3	2.27	0.49
1:B:68:LEU:HD13	1:B:189:GLY:HA3	1.93	0.49
1:B:82:PRO:HD2	1:B:83:ALA:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:TYR:HB2	1:A:276:TYR:CZ	2.48	0.48
1:A:278:GLU:HA	1:A:363:ARG:HH12	1.79	0.48
1:B:106:VAL:CG1	1:B:339:ALA:HB1	2.44	0.48
1:A:284:ALA:HB1	1:A:305:GLY:HA3	1.94	0.48
1:A:338:GLN:HA	1:A:338:GLN:HE21	1.79	0.48
1:A:300:GLU:OE2	1:A:367:HIS:CE1	2.67	0.48
1:A:122:HIS:HE1	1:A:316:SER:O	1.96	0.48
1:A:216:ASP:HA	1:A:217:GLY:HA2	1.60	0.48
1:A:213:LYS:CA	1:A:214:ASP:HB3	2.43	0.47
1:A:369:THR:HB	1:A:391:LEU:HB3	1.97	0.47
1:A:116:THR:O	1:A:183:ARG:CD	2.63	0.46
1:A:222:ASP:HA	1:A:223:PRO:HD3	1.68	0.46
1:A:137:ARG:HH21	1:A:139:LYS:HZ1	1.62	0.46
1:B:248:ILE:HG23	1:B:258:ILE:HD13	1.95	0.46
1:B:122:HIS:CD2	1:B:124:ASP:H	2.21	0.46
1:A:93:VAL:O	1:A:389:ALA:N	2.42	0.46
1:A:361:THR:CG2	1:A:364:GLY:H	2.10	0.46
1:B:95:ALA:H	1:B:96:PRO:CD	2.27	0.46
1:A:109:ILE:HD13	1:A:229:GLU:HG2	1.97	0.46
1:A:356:ASP:O	1:A:367:HIS:HD2	1.99	0.46
1:B:85:THR:O	1:B:87:PRO:HD3	2.16	0.46
1:B:173:VAL:O	1:B:336:LEU:HD11	2.16	0.46
1:B:21:GLU:OE1	1:B:54:MET:HG2	2.16	0.46
1:B:122:HIS:CD2	1:B:123:PRO:HD2	2.51	0.46
1:A:66:ALA:HB3	1:A:196:ILE:CD1	2.46	0.46
1:A:126:ALA:HA	1:A:129:ILE:CD1	2.45	0.45
1:A:273:PRO:O	1:A:274:ALA:C	2.54	0.45
1:A:208:ASP:OD2	1:A:209:GLY:N	2.49	0.45
1:B:131:TRP:HB3	1:B:180:TYR:CD1	2.51	0.45
1:B:230:VAL:CG2	1:B:334:VAL:HG22	2.47	0.45
1:B:48:VAL:O	1:B:52:LYS:HG3	2.17	0.45
1:A:277:PRO:HD2	1:A:278:GLU:OE1	2.17	0.45
1:B:11:SER:HB2	1:B:59:LYS:HB3	1.99	0.45
1:B:352:GLY:HA3	3:B:562:HOH:O	2.17	0.44
1:A:118:VAL:HG22	1:A:181:SER:CB	2.47	0.44
1:B:244:LEU:O	1:B:248:ILE:HG12	2.17	0.44
1:A:213:LYS:CD	1:A:214:ASP:HB3	2.47	0.44
1:A:308:ILE:O	1:A:319:THR:HA	2.17	0.44
1:B:92:ARG:HA	1:B:92:ARG:HD2	1.83	0.44
1:B:352:GLY:HA3	1:B:361:THR:CG2	2.46	0.44
1:A:214:ASP:OD1	1:A:216:ASP:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:SER:OG	1:A:317:TYR:N	2.50	0.44
1:A:89:GLY:CA	1:A:304:PRO:HG2	2.48	0.43
1:A:49:GLY:HA2	1:A:52:LYS:HD3	2.00	0.43
1:A:89:GLY:HA2	1:A:304:PRO:HG2	2.01	0.43
1:A:141:SER:OG	1:A:146:ASP:OD2	2.22	0.43
1:B:338:GLN:CA	1:B:338:GLN:HE21	2.22	0.43
1:B:156:HIS:CD2	1:B:310:SER:HB3	2.54	0.43
1:B:236:GLY:HA2	1:B:272:TYR:O	2.19	0.43
1:B:47:ALA:HB2	3:B:408:HOH:O	2.18	0.43
1:A:352:GLY:HA3	1:A:361:THR:CG2	2.49	0.42
1:A:36:ILE:HG12	1:A:247:MET:HE2	2.01	0.42
1:B:356:ASP:O	1:B:367:HIS:CD2	2.69	0.42
1:B:230:VAL:HA	1:B:257:VAL:O	2.19	0.42
1:A:10:VAL:O	1:A:38:ALA:HA	2.19	0.42
1:A:262:SER:HB2	1:A:282:VAL:O	2.20	0.42
1:A:118:VAL:HG13	1:A:158:ILE:CD1	2.48	0.42
1:A:49:GLY:O	1:A:53:LYS:HE2	2.19	0.42
1:A:61:GLU:HG3	3:A:485:HOH:O	2.18	0.42
1:A:116:THR:O	1:A:183:ARG:HD3	2.19	0.42
1:A:36:ILE:HG12	1:A:247:MET:CE	2.50	0.42
1:B:329:HIS:O	1:B:333:VAL:HG23	2.19	0.42
1:B:122:HIS:HE1	1:B:316:SER:O	2.03	0.42
1:B:359:LYS:O	1:B:365:ILE:HD11	2.20	0.42
1:A:245:TYR:CE1	1:A:278:GLU:OE1	2.66	0.41
1:A:21:GLU:OE1	1:A:55:PRO:HD2	2.19	0.41
1:A:66:ALA:HB3	1:A:196:ILE:HD11	2.02	0.41
1:B:156:HIS:HA	1:B:311:THR:O	2.21	0.41
1:A:297:ARG:HB3	1:A:380:ALA:O	2.21	0.41
1:B:135:THR:HG21	1:B:199:GLY:HA2	2.02	0.41
1:A:321:MET:N	1:A:325:MET:HE2	2.36	0.41
1:A:122:HIS:HB3	1:A:125:LEU:HB2	2.02	0.41
1:B:325:MET:HG2	1:B:325:MET:H	1.66	0.41
1:A:116:THR:O	1:A:183:ARG:HD2	2.21	0.41
1:B:150:GLN:HG3	1:B:183:ARG:NH1	2.37	0.40
1:A:114:LEU:HA	1:A:182:VAL:O	2.21	0.40
1:B:230:VAL:HG22	1:B:334:VAL:HG22	2.02	0.40
1:B:106:VAL:HG11	1:B:339:ALA:HA	2.02	0.40
1:B:300:GLU:HB2	3:B:442:HOH:O	2.22	0.40
1:B:146:ASP:HB3	3:B:487:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	385/398 (97%)	360 (94%)	21 (6%)	4 (1%)	19 28
1	B	377/398 (95%)	348 (92%)	27 (7%)	2 (0%)	34 48
All	All	762/796 (96%)	708 (93%)	48 (6%)	6 (1%)	24 35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	ASP
1	A	210	VAL
1	A	216	ASP
1	B	82	PRO
1	A	119	ASP
1	B	375	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	300/306 (98%)	268 (89%)	32 (11%)	8 11
1	B	298/306 (97%)	271 (91%)	27 (9%)	12 17
All	All	598/612 (98%)	539 (90%)	59 (10%)	10 14

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	12	VAL
1	A	14	LYS
1	A	22	VAL
1	A	46	ASN
1	A	48	VAL
1	A	61	GLU
1	A	65	GLN
1	A	68	LEU
1	A	75	LEU
1	A	91	GLU
1	A	118	VAL
1	A	133	VAL
1	A	142	THR
1	A	145	ARG
1	A	147	CYS
1	A	161	ILE
1	A	177	VAL
1	A	183	ARG
1	A	213	LYS
1	A	214	ASP
1	A	216	ASP
1	A	218	ILE
1	A	246	ASP
1	A	262	SER
1	A	325	MET
1	A	334	VAL
1	A	359	LYS
1	A	361	THR
1	A	387	VAL
1	A	388	ARG
1	A	391	LEU
1	B	3	GLN
1	B	21	GLU
1	B	51	LEU
1	B	53	LYS
1	B	67	VAL
1	B	68	LEU
1	B	73	SER
1	B	93	VAL
1	B	106	VAL
1	B	108	VAL
1	B	115	ASP

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Mol	Chain	Res	Type
1	B	121	ASP
1	B	133	VAL
1	B	142	THR
1	B	150	GLN
1	B	188	ARG
1	B	235	LEU
1	B	271	SER
1	B	325	MET
1	B	334	VAL
1	B	338	GLN
1	B	347	LYS
1	B	351	VAL
1	B	356	ASP
1	B	361	THR
1	B	376	THR
1	B	388	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	122	HIS
1	A	150	GLN
1	A	296	ASN
1	A	338	GLN
1	A	367	HIS
1	A	394	GLN
1	B	3	GLN
1	B	4	ASN
1	B	64	HIS
1	B	65	GLN
1	B	122	HIS
1	B	296	ASN
1	B	338	GLN
1	B	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 11 ligands modelled in this entry, 11 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

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, 95^{th} 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	389/398 (97%)	-0.68	1 (0%)	94	94	12, 21, 39, 49	0
1	B	383/398 (96%)	-0.65	1 (0%)	94	94	13, 22, 37, 49	0
All	All	772/796 (96%)	-0.66	2 (0%)	94	94	12, 22, 39, 49	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	20	HIS	2.8
1	A	214	ASP	2.7

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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, 95^{th} 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	A	400	1/1	0.99	0.11	2.88	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CA	A	401	1/1	0.99	0.09	-0.33	26,26,26,26	0
2	CA	B	400	1/1	0.96	0.07	-1.59	33,33,33,33	0
2	CA	A	403	1/1	0.97	0.05	-1.99	49,49,49,49	0
2	CA	A	404	1/1	0.99	0.04	-2.42	28,28,28,28	0
2	CA	A	399	1/1	1.00	0.05	-2.47	21,21,21,21	0
2	CA	B	399	1/1	0.98	0.05	-2.73	29,29,29,29	0
2	CA	B	402	1/1	0.99	0.06	-2.85	17,17,17,17	0
2	CA	B	403	1/1	1.00	0.05	-3.35	19,19,19,19	0
2	CA	A	402	1/1	0.99	0.02	-5.02	31,31,31,31	0
2	CA	B	401	1/1	0.99	0.09	-	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.