Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:27 PM GMT

PDB ID	:	5AJL
Title	:	Sdsa sulfatase tetragonal
Authors	:	De la Mora, E.; Flores-Hernandez, E.; Jakoncic, J.; Stojanoff, V.; Sanchez-Puig, N.; Moreno, A.
Deposited on	:	2015-02-25
Resolution	:	3.45 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 ⓘ symbol.

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

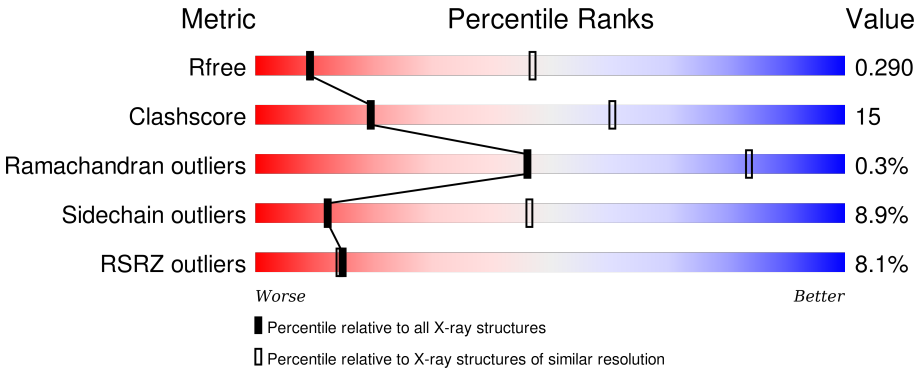
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 3.45 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	1000 (3.56-3.36)
Clashscore	102246	1090 (3.56-3.36)
Ramachandran outliers	100387	1057 (3.56-3.36)
Sidechain outliers	100360	1058 (3.56-3.36)
RSRZ outliers	91569	1005 (3.56-3.36)

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	658	9% 77% 16%
1	B	658	7% 74% 19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9846 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 ALKYL SULFATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	631	Total	C	N	O	S	0	0	1
			4921	3105	890	916	10			
1	B	631	Total	C	N	O	S	0	0	1
			4921	3105	890	916	10			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

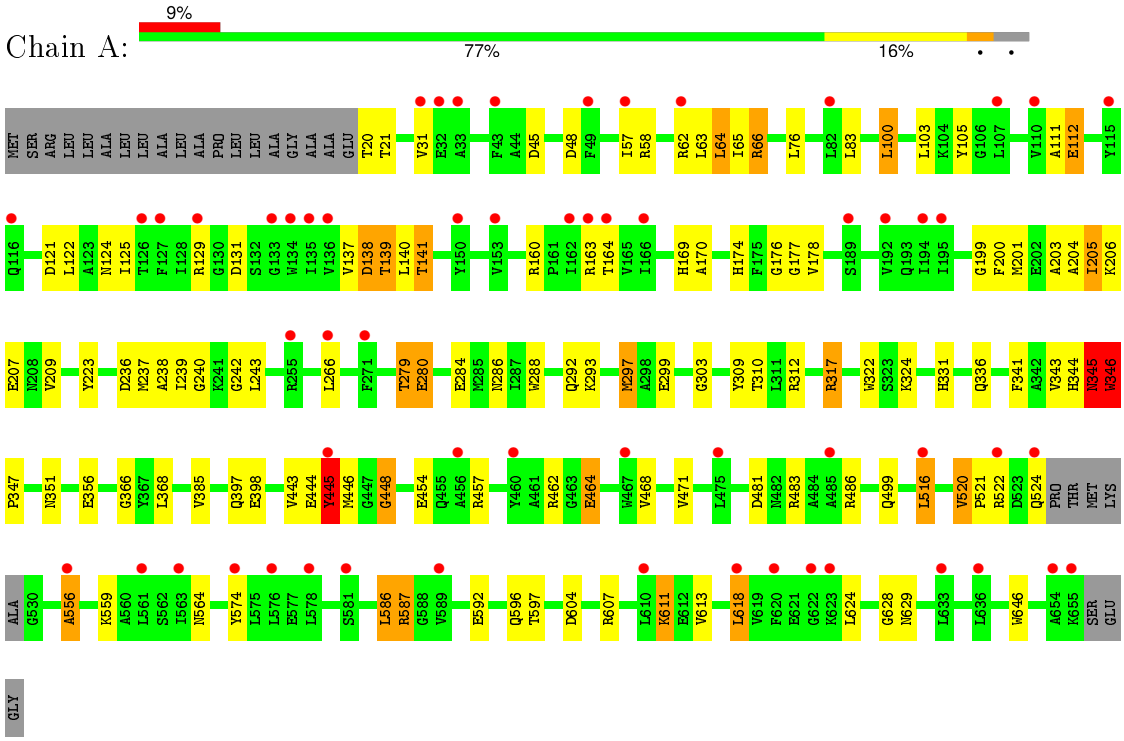
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

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.

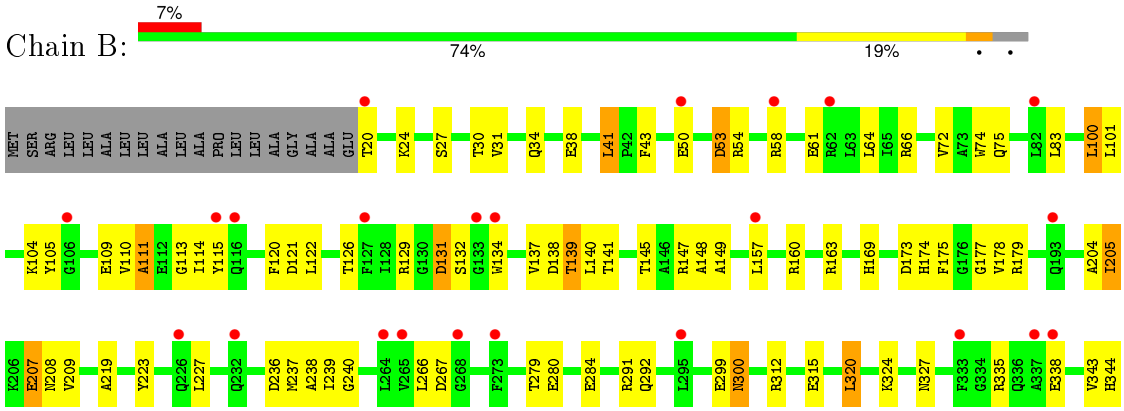
- Molecule 1: ALKYL SULFATASE

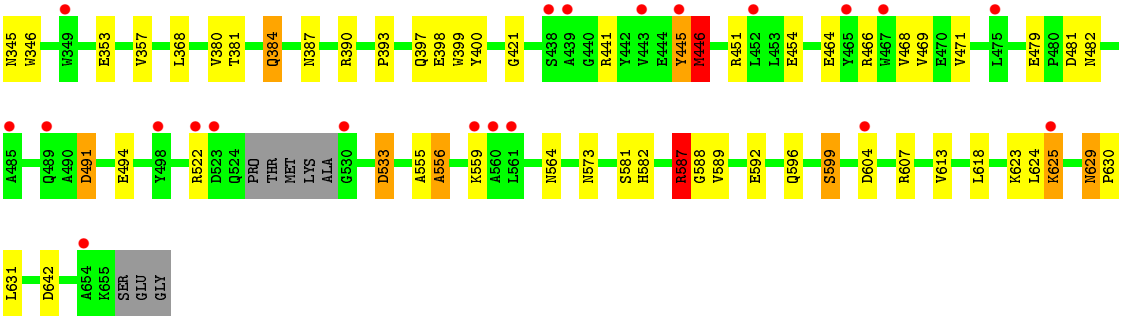
Chain A:



- Molecule 1: ALKYL SULFATASE

Chain B:




N345 W346 W349 E353 V357 L368 V380 T381 Q384 N387 R390 P393 Q397 E398 W399 Y400 G421 S438 A439 G440 R441 Y442 V443 E444 Y445 N446 R451 L452 L453 E454 E464 Y465 R466 W467 V468 V469 E470 V471 L475 E479 P480 D481 N482
A485 Q489 A490 D491 E494 Y498 R522 D523 Q524 PRO THR MET LYS ALA G530 D533 A555 A556 K559 A560 L561 N564 N573 S581 H582 R587 G588 V589 E592 Q596 S599 D604 R607 V613 L618 K623 L624 K625 N629 P630
L631 D642 A654 K655 SER GLU GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	88.58Å 88.58Å 193.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.61 – 3.45 52.61 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (52.61-3.45) 99.8 (52.61-3.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.244 , 0.289 0.248 , 0.290	Depositor DCC
R_{free} test set	1005 reflections (5.40%)	DCC
Wilson B-factor (Å^2)	106.6	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 66.9	EDS
Estimated twinning fraction	0.065 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 19623 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9846	wwPDB-VP
Average B, all atoms (Å^2)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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: ZN

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	0.47	1/5028 (0.0%)	0.74	7/6829 (0.1%)
1	B	0.46	0/5028	0.73	4/6829 (0.1%)
All	All	0.47	1/10056 (0.0%)	0.73	11/13658 (0.1%)

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	6
1	B	0	11
All	All	0	17

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	524	GLN	C-O	5.98	1.34	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	41	LEU	CA-CB-CG	7.64	132.86	115.30
1	B	100	LEU	CA-CB-CG	7.54	132.65	115.30
1	A	618	LEU	CA-CB-CG	6.97	131.34	115.30
1	A	520	VAL	C-N-CD	6.68	142.42	128.40
1	B	629	ASN	C-N-CD	6.42	141.87	128.40
1	A	346	TRP	C-N-CD	5.87	140.74	128.40
1	A	100	LEU	CA-CB-CG	5.86	128.78	115.30
1	A	112	GLU	N-CA-C	-5.47	96.23	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	317	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	516	LEU	CA-CB-CG	5.09	127.01	115.30
1	B	451	ARG	NE-CZ-NH1	5.05	122.82	120.30

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	ILE	Peptide
1	A	345	ASN	Peptide
1	A	444	GLU	Peptide
1	A	445	TYR	Peptide
1	A	448	GLY	Peptide
1	A	556	ALA	Peptide
1	B	110	VAL	Peptide
1	B	111	ALA	Peptide
1	B	205	ILE	Peptide
1	B	207	GLU	Peptide
1	B	208	ASN	Peptide
1	B	345	ASN	Peptide
1	B	384	GLN	Peptide
1	B	446	MET	Peptide
1	B	53	ASP	Peptide
1	B	556	ALA	Peptide
1	B	587	ARG	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	4921	0	4824	147	1
1	B	4921	0	4823	159	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
All	All	9846	0	9647	292	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 15.

All (292) 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:111:ALA:CB	1:B:114:ILE:HB	1.46	1.45
1:B:223:TYR:CD1	1:B:237:MET:HE2	1.55	1.39
1:B:223:TYR:CD1	1:B:237:MET:CE	2.06	1.38
1:A:223:TYR:CD1	1:A:237:MET:HE2	1.58	1.37
1:B:174:HIS:CE1	1:B:344:HIS:CE1	2.16	1.34
1:B:174:HIS:CE1	1:B:344:HIS:HE1	1.48	1.29
1:B:126:THR:HB	1:B:137:VAL:CG2	1.63	1.28
1:B:111:ALA:HB2	1:B:114:ILE:CB	1.63	1.27
1:A:174:HIS:CE1	1:A:344:HIS:HE2	1.57	1.23
1:A:223:TYR:CD1	1:A:237:MET:CE	2.20	1.22
1:A:64:LEU:HD12	1:A:65:ILE:N	1.55	1.22
1:B:126:THR:HB	1:B:137:VAL:HG22	1.19	1.17
1:A:121:ASP:CG	1:A:141:THR:OG1	1.82	1.16
1:B:120:PHE:HE2	1:B:149:ALA:N	1.44	1.14
1:B:111:ALA:HB3	1:B:114:ILE:N	1.61	1.14
1:B:111:ALA:CB	1:B:114:ILE:CB	2.18	1.13
1:B:126:THR:CB	1:B:137:VAL:CG2	2.29	1.11
1:A:174:HIS:CE1	1:A:344:HIS:NE2	2.17	1.10
1:B:174:HIS:HE1	1:B:344:HIS:CE1	1.59	1.08
1:A:596:GLN:HG3	1:A:629:ASN:O	1.53	1.08
1:B:630:PRO:HD2	1:B:631:LEU:HG	1.23	1.08
1:B:111:ALA:HB3	1:B:114:ILE:H	0.99	1.07
1:A:293:LYS:HD3	1:A:336:GLN:O	1.53	1.07
1:B:139:THR:OG1	1:B:177:GLY:C	1.93	1.07
1:A:303:GLY:H	1:A:345:ASN:ND2	1.55	1.03
1:B:573:ASN:O	1:B:588:GLY:N	1.90	1.03
1:A:121:ASP:OD2	1:A:141:THR:CB	2.08	1.02
1:B:292:GLN:OE1	1:B:292:GLN:N	1.90	1.02
1:B:398:GLU:OE1	1:B:400:TYR:OH	1.75	1.02
1:B:163:ARG:NH1	1:B:267:ASP:OD2	1.92	1.00
1:B:120:PHE:CE2	1:B:149:ALA:N	2.31	0.98
1:B:139:THR:HG1	1:B:177:GLY:C	1.68	0.96
1:B:381:THR:H	1:B:384:GLN:HG3	1.28	0.96
1:B:111:ALA:CB	1:B:114:ILE:H	1.79	0.95
1:B:381:THR:OG1	1:B:384:GLN:HG2	1.67	0.95
1:A:586:LEU:HD13	1:B:327:ASN:ND2	1.79	0.95
1:B:140:LEU:O	1:B:173:ASP:O	1.84	0.94
1:B:239:ILE:HD12	1:B:344:HIS:CD2	2.02	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:ILE:HD12	1:B:344:HIS:HD2	1.31	0.94
1:A:125:ILE:HB	1:A:140:LEU:HD11	1.49	0.93
1:A:121:ASP:OD1	1:A:122:LEU:N	2.03	0.92
1:B:122:LEU:HD12	1:B:240:GLY:HA3	1.51	0.92
1:B:223:TYR:CD1	1:B:237:MET:HE3	2.02	0.92
1:B:126:THR:CB	1:B:137:VAL:HG21	1.96	0.91
1:B:126:THR:HB	1:B:137:VAL:HG21	1.53	0.91
1:B:111:ALA:CB	1:B:114:ILE:N	2.32	0.91
1:A:286:ASN:ND2	1:A:297:MET:HE1	1.85	0.90
1:A:112:GLU:O	1:A:292:GLN:HG2	1.70	0.90
1:A:236:ASP:OD1	1:A:237:MET:N	2.05	0.89
1:B:223:TYR:CE1	1:B:237:MET:HE3	2.08	0.87
1:A:310:THR:OG1	1:A:312:ARG:HG2	1.74	0.87
1:A:239:ILE:HD12	1:A:344:HIS:ND1	1.89	0.86
1:B:121:ASP:OD1	1:B:122:LEU:N	2.09	0.86
1:A:223:TYR:HD1	1:A:237:MET:HE2	1.05	0.85
1:A:140:LEU:O	1:A:177:GLY:N	2.09	0.85
1:A:174:HIS:HE1	1:A:344:HIS:CD2	1.93	0.85
1:B:126:THR:OG1	1:B:137:VAL:HG21	1.76	0.85
1:A:445:TYR:CD1	1:B:446:MET:HE1	2.11	0.85
1:B:111:ALA:HB3	1:B:114:ILE:CA	2.07	0.85
1:A:280:GLU:HB2	1:A:299:GLU:HB3	1.58	0.84
1:B:140:LEU:O	1:B:173:ASP:C	2.15	0.84
1:B:111:ALA:CB	1:B:114:ILE:CA	2.56	0.82
1:B:223:TYR:HD1	1:B:237:MET:HE2	1.05	0.82
1:B:381:THR:OG1	1:B:384:GLN:CG	2.26	0.82
1:A:445:TYR:CD1	1:B:446:MET:CE	2.64	0.79
1:B:596:GLN:HG3	1:B:629:ASN:O	1.81	0.79
1:B:140:LEU:HD23	1:B:145:THR:HB	1.63	0.79
1:A:303:GLY:N	1:A:345:ASN:ND2	2.31	0.78
1:B:223:TYR:CE1	1:B:237:MET:CE	2.65	0.78
1:B:163:ARG:NH1	1:B:267:ASP:CG	2.38	0.77
1:A:236:ASP:OD1	1:A:240:GLY:O	2.01	0.77
1:A:223:TYR:CD1	1:A:237:MET:HE3	2.20	0.77
1:A:205:ILE:O	1:A:207:GLU:N	2.18	0.77
1:A:303:GLY:H	1:A:345:ASN:HD22	1.32	0.76
1:A:169:HIS:NE2	1:A:299:GLU:OE1	2.18	0.76
1:A:310:THR:HG23	1:A:312:ARG:HG3	1.66	0.76
1:A:140:LEU:N	1:A:140:LEU:HD12	2.00	0.76
1:B:398:GLU:OE1	1:B:400:TYR:CZ	2.38	0.75
1:A:445:TYR:HD1	1:B:446:MET:HE1	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:HIS:CE1	1:A:344:HIS:CD2	2.72	0.73
1:B:132:SER:OG	1:B:163:ARG:NH1	2.22	0.72
1:B:205:ILE:HD13	1:B:205:ILE:N	2.04	0.72
1:A:286:ASN:CG	1:A:297:MET:HE3	2.11	0.72
1:A:303:GLY:N	1:A:345:ASN:HD22	1.88	0.71
1:A:286:ASN:ND2	1:A:297:MET:CE	2.53	0.71
1:A:64:LEU:CD1	1:A:65:ILE:N	2.46	0.71
1:A:445:TYR:CE1	1:B:446:MET:HE3	2.26	0.70
1:A:64:LEU:HD12	1:A:65:ILE:CA	2.20	0.70
1:A:223:TYR:HA	1:A:237:MET:HE1	1.73	0.70
1:B:120:PHE:CE2	1:B:149:ALA:CA	2.75	0.70
1:A:174:HIS:NE2	1:A:344:HIS:NE2	2.32	0.70
1:B:126:THR:CB	1:B:137:VAL:HG22	2.05	0.69
1:A:64:LEU:HD12	1:A:65:ILE:C	2.11	0.69
1:A:280:GLU:CB	1:A:299:GLU:HB3	2.21	0.69
1:A:310:THR:CG2	1:A:312:ARG:HG3	2.22	0.69
1:A:286:ASN:CG	1:A:297:MET:CE	2.61	0.69
1:A:586:LEU:CD1	1:B:327:ASN:ND2	2.55	0.68
1:B:464:GLU:O	1:B:468:VAL:HG23	1.94	0.67
1:A:279:THR:HG22	1:A:322:TRP:CG	2.30	0.67
1:B:174:HIS:NE2	1:B:299:GLU:OE2	2.21	0.67
1:A:611:LYS:HD2	1:A:611:LYS:C	2.14	0.67
1:B:132:SER:OG	1:B:163:ARG:NH2	2.24	0.67
1:A:464:GLU:O	1:A:468:VAL:HG23	1.94	0.66
1:A:64:LEU:C	1:A:64:LEU:HD12	2.16	0.66
1:A:200:PHE:HD2	1:A:201:MET:HG2	1.60	0.66
1:B:280:GLU:HB3	1:B:284:GLU:OE1	1.95	0.66
1:A:223:TYR:CE1	1:A:237:MET:HE3	2.31	0.65
1:A:48:ASP:HB3	1:A:346:TRP:CZ2	2.31	0.65
1:A:124:ASN:ND2	1:A:345:ASN:O	2.28	0.65
1:A:293:LYS:CD	1:A:336:GLN:O	2.39	0.65
1:B:573:ASN:O	1:B:588:GLY:CA	2.45	0.64
1:B:174:HIS:NE2	1:B:344:HIS:CE1	2.64	0.64
1:B:126:THR:H	1:B:137:VAL:HG23	1.61	0.64
1:A:223:TYR:HA	1:A:237:MET:CE	2.27	0.64
1:B:74:TRP:CE2	1:B:120:PHE:O	2.51	0.64
1:A:205:ILE:O	1:A:206:LYS:C	2.35	0.64
1:A:139:THR:OG1	1:A:178:VAL:N	2.30	0.64
1:B:139:THR:OG1	1:B:178:VAL:N	2.29	0.64
1:A:121:ASP:OD2	1:A:141:THR:OG1	0.65	0.63
1:A:201:MET:O	1:A:204:ALA:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:GLY:H	1:A:345:ASN:HD21	1.44	0.63
1:A:310:THR:OG1	1:A:312:ARG:CG	2.47	0.63
1:B:204:ALA:HB3	1:B:205:ILE:HD13	1.80	0.62
1:A:443:VAL:O	1:A:448:GLY:N	2.33	0.62
1:B:111:ALA:HB2	1:B:114:ILE:HB	0.68	0.62
1:B:343:VAL:O	1:B:344:HIS:ND1	2.23	0.61
1:B:380:VAL:HG13	1:B:384:GLN:HB2	1.81	0.61
1:B:630:PRO:HD2	1:B:631:LEU:CG	2.15	0.61
1:A:397:GLN:O	1:A:398:GLU:HG2	2.01	0.61
1:A:343:VAL:O	1:A:344:HIS:HD2	1.84	0.60
1:B:126:THR:OG1	1:B:137:VAL:CG2	2.41	0.60
1:B:163:ARG:HH12	1:B:267:ASP:CG	2.04	0.59
1:B:381:THR:N	1:B:384:GLN:HG3	2.09	0.59
1:B:223:TYR:CG	1:B:237:MET:HE2	2.29	0.59
1:A:205:ILE:HD13	1:A:205:ILE:N	2.17	0.59
1:A:200:PHE:CD2	1:A:201:MET:HG2	2.37	0.59
1:B:132:SER:OG	1:B:163:ARG:CZ	2.51	0.58
1:A:611:LYS:HD2	1:A:611:LYS:O	2.02	0.58
1:B:111:ALA:CB	1:B:114:ILE:CG1	2.82	0.58
1:A:445:TYR:CE1	1:B:446:MET:CE	2.88	0.57
1:A:237:MET:O	1:A:238:ALA:HB3	2.05	0.56
1:B:120:PHE:HE2	1:B:148:ALA:C	2.06	0.56
1:B:111:ALA:HB1	1:B:114:ILE:HG13	1.87	0.56
1:A:137:VAL:O	1:A:138:ASP:HB2	2.06	0.56
1:A:279:THR:CG2	1:A:322:TRP:HA	2.36	0.56
1:B:109:GLU:OE2	1:B:111:ALA:O	2.24	0.56
1:A:586:LEU:CD1	1:B:327:ASN:HD22	2.18	0.56
1:B:111:ALA:HB1	1:B:114:ILE:CB	2.30	0.56
1:A:556:ALA:O	1:A:559:LYS:HG3	2.06	0.56
1:B:111:ALA:HB1	1:B:114:ILE:CG1	2.36	0.56
1:A:443:VAL:O	1:A:448:GLY:HA2	2.06	0.56
1:B:137:VAL:O	1:B:138:ASP:HB2	2.06	0.55
1:B:205:ILE:HG22	1:B:209:VAL:HG21	1.89	0.55
1:B:139:THR:HG21	1:B:178:VAL:HB	1.87	0.55
1:A:462:ARG:HB2	1:A:464:GLU:HG2	1.87	0.55
1:B:280:GLU:HB2	1:B:299:GLU:HB3	1.88	0.55
1:B:121:ASP:OD2	1:B:141:THR:OG1	2.18	0.55
1:A:443:VAL:HG12	1:A:448:GLY:HA2	1.88	0.55
1:A:111:ALA:O	1:A:112:GLU:C	2.44	0.55
1:A:201:MET:O	1:A:204:ALA:HB3	2.06	0.54
1:A:236:ASP:CG	1:A:238:ALA:H	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:GLY:O	1:A:629:ASN:C	2.43	0.54
1:B:120:PHE:HE2	1:B:149:ALA:H	1.46	0.54
1:B:381:THR:OG1	1:B:384:GLN:HG3	2.08	0.54
1:B:204:ALA:CB	1:B:205:ILE:HD13	2.37	0.54
1:A:57:ILE:O	1:A:58:ARG:HG3	2.07	0.54
1:A:112:GLU:O	1:A:292:GLN:CG	2.51	0.54
1:A:64:LEU:CD1	1:A:65:ILE:C	2.76	0.54
1:B:169:HIS:NE2	1:B:280:GLU:OE1	2.40	0.54
1:A:139:THR:C	1:A:140:LEU:HD12	2.29	0.54
1:B:219:ALA:HB2	1:B:312:ARG:HG3	1.89	0.54
1:A:164:THR:HG21	1:A:266:LEU:HD13	1.91	0.53
1:B:74:TRP:CD2	1:B:120:PHE:O	2.61	0.53
1:B:381:THR:H	1:B:384:GLN:CG	2.13	0.53
1:A:170:ALA:HB1	1:A:204:ALA:HA	1.91	0.53
1:B:223:TYR:HA	1:B:237:MET:CE	2.38	0.53
1:B:387:ASN:OD1	1:B:466:ARG:NH2	2.42	0.53
1:A:446:MET:HA	1:B:446:MET:HA	1.89	0.52
1:B:120:PHE:CE2	1:B:148:ALA:C	2.83	0.52
1:B:223:TYR:CG	1:B:237:MET:CE	2.86	0.52
1:A:279:THR:HG22	1:A:322:TRP:CD2	2.44	0.52
1:A:341:PHE:HB3	1:A:347:PRO:HB3	1.91	0.52
1:B:291:ARG:C	1:B:292:GLN:OE1	2.48	0.52
1:A:64:LEU:CD1	1:A:65:ILE:O	2.58	0.52
1:A:64:LEU:HD21	1:A:66:ARG:HH11	1.74	0.52
1:B:113:GLY:HA2	1:B:129:ARG:HD2	1.92	0.52
1:B:137:VAL:O	1:B:137:VAL:HG23	2.10	0.52
1:A:471:VAL:HG21	1:B:445:TYR:CE2	2.45	0.52
1:A:205:ILE:HG22	1:A:209:VAL:HG21	1.92	0.52
1:B:479:GLU:HB3	1:B:482:ASN:HB2	1.92	0.52
1:B:380:VAL:CG1	1:B:384:GLN:HB2	2.40	0.51
1:B:120:PHE:CD2	1:B:149:ALA:HB2	2.46	0.51
1:A:64:LEU:HD12	1:A:65:ILE:H	1.60	0.51
1:B:380:VAL:HG13	1:B:384:GLN:CB	2.40	0.51
1:A:443:VAL:O	1:A:448:GLY:CA	2.59	0.51
1:A:293:LYS:O	1:A:293:LYS:HG2	2.10	0.51
1:B:236:ASP:OD2	1:B:238:ALA:N	2.43	0.51
1:A:521:PRO:HD2	1:A:646:TRP:CE3	2.46	0.50
1:B:393:PRO:O	1:B:397:GLN:HB2	2.12	0.50
1:A:279:THR:HG21	1:A:322:TRP:HA	1.94	0.50
1:A:169:HIS:CE1	1:A:299:GLU:HB2	2.47	0.50
1:A:169:HIS:HE2	1:A:299:GLU:CD	2.13	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:MET:HB2	1:A:242:GLY:HA2	1.94	0.50
1:B:204:ALA:C	1:B:205:ILE:HD13	2.32	0.50
1:B:169:HIS:CD2	1:B:280:GLU:OE1	2.64	0.49
1:B:204:ALA:HB3	1:B:205:ILE:CD1	2.42	0.49
1:A:64:LEU:HD21	1:A:66:ARG:NH1	2.27	0.49
1:B:74:TRP:CD1	1:B:120:PHE:O	2.65	0.49
1:B:140:LEU:CD2	1:B:145:THR:HB	2.37	0.49
1:B:53:ASP:OD1	1:B:104:LYS:HE3	2.12	0.49
1:A:596:GLN:CG	1:A:629:ASN:O	2.42	0.49
1:A:303:GLY:CA	1:A:345:ASN:HD22	2.24	0.49
1:A:303:GLY:CA	1:A:345:ASN:ND2	2.76	0.49
1:A:139:THR:N	1:A:174:HIS:O	2.29	0.49
1:A:279:THR:CG2	1:A:322:TRP:CG	2.95	0.49
1:A:239:ILE:HD12	1:A:344:HIS:CE1	2.48	0.49
1:B:139:THR:OG1	1:B:177:GLY:CA	2.61	0.48
1:B:139:THR:OG1	1:B:139:THR:O	2.29	0.48
1:B:139:THR:HG21	1:B:178:VAL:CB	2.44	0.48
1:B:596:GLN:CG	1:B:629:ASN:O	2.58	0.47
1:B:27:SER:O	1:B:31:VAL:HG23	2.14	0.47
1:B:205:ILE:O	1:B:207:GLU:N	2.47	0.47
1:A:140:LEU:CD1	1:A:140:LEU:N	2.73	0.47
1:B:121:ASP:O	1:B:122:LEU:C	2.53	0.47
1:B:604:ASP:HA	1:B:607:ARG:HB2	1.96	0.47
1:B:24:LYS:NZ	1:B:491:ASP:OD2	2.48	0.47
1:A:280:GLU:HB3	1:A:284:GLU:OE1	2.15	0.47
1:A:604:ASP:HA	1:A:607:ARG:HG3	1.96	0.46
1:A:63:LEU:HD12	1:A:63:LEU:HA	1.75	0.46
1:A:169:HIS:NE2	1:A:280:GLU:OE2	2.48	0.46
1:A:343:VAL:O	1:A:344:HIS:CD2	2.67	0.46
1:A:310:THR:CG2	1:A:312:ARG:CG	2.94	0.46
1:A:288:TRP:HH2	1:A:293:LYS:HG3	1.79	0.46
1:B:599:SER:HB3	1:B:625:LYS:HG3	1.96	0.45
1:A:76:LEU:HD13	1:A:105:TYR:CD2	2.51	0.45
1:A:223:TYR:CE1	1:A:237:MET:CE	2.83	0.45
1:A:139:THR:C	1:A:140:LEU:CD1	2.86	0.45
1:A:141:THR:CG2	1:A:243:LEU:HD11	2.47	0.45
1:B:120:PHE:CE2	1:B:148:ALA:HB3	2.52	0.45
1:B:346:TRP:O	1:B:346:TRP:CD1	2.70	0.45
1:B:74:TRP:CG	1:B:120:PHE:O	2.71	0.44
1:B:205:ILE:HG22	1:B:209:VAL:CG2	2.47	0.44
1:A:48:ASP:CG	1:A:346:TRP:HZ2	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:PHE:HB3	1:B:399:TRP:CZ2	2.52	0.44
1:A:140:LEU:O	1:A:176:GLY:CA	2.65	0.44
1:A:48:ASP:HB3	1:A:346:TRP:HZ2	1.78	0.44
1:B:140:LEU:HD23	1:B:145:THR:CB	2.40	0.44
1:A:564:ASN:HB3	1:A:597:THR:HA	1.99	0.44
1:A:303:GLY:HA3	1:A:345:ASN:HD22	1.80	0.44
1:A:345:ASN:N	1:A:345:ASN:OD1	2.51	0.44
1:B:236:ASP:OD2	1:B:238:ALA:HA	2.18	0.44
1:B:300:ASN:OD1	1:B:300:ASN:N	2.51	0.43
1:B:587:ARG:O	1:B:589:VAL:N	2.51	0.43
1:B:353:GLU:O	1:B:357:VAL:HG23	2.18	0.43
1:B:139:THR:HG23	1:B:175:PHE:HA	2.00	0.43
1:A:397:GLN:O	1:A:398:GLU:CG	2.66	0.43
1:A:141:THR:HG21	1:A:243:LEU:CD1	2.49	0.43
1:A:303:GLY:HA3	1:A:345:ASN:ND2	2.33	0.43
1:A:286:ASN:OD1	1:A:297:MET:HE3	2.19	0.43
1:B:320:LEU:HD11	1:B:324:LYS:HE2	2.00	0.43
1:A:309:TYR:CE1	1:B:421:GLY:HA3	2.54	0.43
1:A:574:TYR:CE1	1:A:587:ARG:HB2	2.54	0.43
1:B:120:PHE:CE2	1:B:149:ALA:HA	2.51	0.42
1:B:134:TRP:NE1	1:B:160:ARG:HB2	2.34	0.42
1:B:573:ASN:O	1:B:588:GLY:HA2	2.19	0.42
1:A:443:VAL:CG1	1:A:448:GLY:HA2	2.48	0.42
1:A:346:TRP:CD1	1:A:346:TRP:C	2.93	0.42
1:B:629:ASN:OD1	1:B:631:LEU:N	2.33	0.42
1:A:199:GLY:O	1:A:203:ALA:HB2	2.20	0.42
1:B:564:ASN:N	1:B:564:ASN:HD22	2.16	0.42
1:B:139:THR:N	1:B:174:HIS:O	2.26	0.42
1:B:555:ALA:O	1:B:559:LYS:HE3	2.20	0.42
1:B:223:TYR:HD1	1:B:237:MET:CE	1.79	0.42
1:A:48:ASP:CB	1:A:346:TRP:HZ2	2.32	0.42
1:A:236:ASP:CG	1:A:237:MET:N	2.72	0.42
1:A:139:THR:OG1	1:A:178:VAL:CA	2.68	0.42
1:B:533:ASP:N	1:B:533:ASP:OD1	2.45	0.41
1:B:556:ALA:HB1	1:B:581:SER:HA	2.02	0.41
1:B:120:PHE:CE2	1:B:149:ALA:HB2	2.56	0.41
1:A:63:LEU:HD21	1:A:65:ILE:HD11	2.02	0.41
1:A:345:ASN:HB2	1:A:346:TRP:H	1.60	0.41
1:A:297:MET:HE3	1:A:297:MET:HA	2.02	0.41
1:A:445:TYR:CE1	1:B:471:VAL:HG21	2.56	0.41
1:A:366:GLY:HA3	1:B:582:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:THR:O	1:B:34:GLN:HG2	2.21	0.41
1:B:126:THR:N	1:B:137:VAL:HG23	2.34	0.40
1:A:446:MET:HA	1:B:446:MET:SD	2.62	0.40
1:B:121:ASP:OD2	1:B:141:THR:CB	2.69	0.40
1:B:115:TYR:CE2	1:B:157:LEU:HD13	2.56	0.40
1:B:74:TRP:NE1	1:B:120:PHE:O	2.54	0.40
1:B:466:ARG:HA	1:B:469:VAL:HG22	2.04	0.40
1:A:520:VAL:HG23	1:A:520:VAL:O	2.21	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)
1:A:62:ARG:NH1	1:B:587:ARG:NH1[3_554]	2.16	0.04

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	627/658 (95%)	592 (94%)	32 (5%)	3 (0%)	34 77
1	B	627/658 (95%)	586 (94%)	40 (6%)	1 (0%)	52 87
All	All	1254/1316 (95%)	1178 (94%)	72 (6%)	4 (0%)	46 84

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	280	GLU
1	B	131	ASP
1	A	138	ASP
1	A	385	VAL

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	499/521 (96%)	457 (92%)	42 (8%)	14 49
1	B	499/521 (96%)	452 (91%)	47 (9%)	11 43
All	All	998/1042 (96%)	909 (91%)	89 (9%)	12 46

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	21	THR
1	A	31	VAL
1	A	45	ASP
1	A	64	LEU
1	A	66	ARG
1	A	83	LEU
1	A	100	LEU
1	A	103	LEU
1	A	129	ARG
1	A	131	ASP
1	A	139	THR
1	A	141	THR
1	A	160	ARG
1	A	163	ARG
1	A	279	THR
1	A	297	MET
1	A	317	ARG
1	A	324	LYS
1	A	331	HIS
1	A	345	ASN
1	A	346	TRP
1	A	351	ASN
1	A	356	GLU
1	A	368	LEU
1	A	445	TYR
1	A	454	GLU

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Mol	Chain	Res	Type
1	A	457	ARG
1	A	464	GLU
1	A	481	ASP
1	A	483	ARG
1	A	486	ARG
1	A	499	GLN
1	A	516	LEU
1	A	522	ARG
1	A	586	LEU
1	A	587	ARG
1	A	592	GLU
1	A	611	LYS
1	A	613	VAL
1	A	618	LEU
1	A	624	LEU
1	B	20	THR
1	B	38	GLU
1	B	41	LEU
1	B	50	GLU
1	B	54	ARG
1	B	58	ARG
1	B	61	GLU
1	B	64	LEU
1	B	66	ARG
1	B	72	VAL
1	B	75	GLN
1	B	83	LEU
1	B	100	LEU
1	B	101	LEU
1	B	105	TYR
1	B	131	ASP
1	B	139	THR
1	B	147	ARG
1	B	179	ARG
1	B	227	LEU
1	B	266	LEU
1	B	279	THR
1	B	300	ASN
1	B	315	GLU
1	B	320	LEU
1	B	335	ARG
1	B	338	GLU

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Mol	Chain	Res	Type
1	B	368	LEU
1	B	390	ARG
1	B	441	ARG
1	B	445	TYR
1	B	446	MET
1	B	454	GLU
1	B	481	ASP
1	B	491	ASP
1	B	494	GLU
1	B	522	ARG
1	B	533	ASP
1	B	587	ARG
1	B	592	GLU
1	B	599	SER
1	B	613	VAL
1	B	618	LEU
1	B	623	LYS
1	B	624	LEU
1	B	625	LYS
1	B	642	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	345	ASN
1	A	473	ASN
1	B	455	GLN
1	B	473	ASN
1	B	564	ASN
1	B	590	GLN

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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 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

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	631/658 (95%)	0.62	58 (9%)	11	11	77, 128, 168, 197	0
1	B	631/658 (95%)	0.57	44 (6%)	19	18	81, 128, 176, 204	0
All	All	1262/1316 (95%)	0.60	102 (8%)	15	14	77, 128, 172, 204	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	654	ALA	5.9
1	A	655	LYS	4.9
1	A	524	GLN	4.5
1	B	530	GLY	4.0
1	B	133	GLY	3.7
1	A	610	LEU	3.7
1	A	134	TRP	3.6
1	A	57	ILE	3.6
1	A	136	VAL	3.4
1	A	162	ILE	3.4
1	A	164	THR	3.4
1	A	623	LYS	3.4
1	A	195	ILE	3.4
1	A	82	LEU	3.2
1	B	452	LEU	3.2
1	A	107	LEU	3.2
1	A	522	ARG	3.2
1	A	129	ARG	3.1
1	A	135	ILE	3.1
1	B	445	TYR	3.1
1	A	271	PHE	3.1
1	A	563	ILE	3.0
1	A	192	VAL	2.9
1	B	106	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	578	LEU	2.8
1	B	338	GLU	2.8
1	A	460	TYR	2.8
1	A	622	GLY	2.8
1	A	163	ARG	2.8
1	B	58	ARG	2.8
1	A	266	LEU	2.8
1	B	443	VAL	2.7
1	B	560	ALA	2.7
1	B	82	LEU	2.7
1	A	561	LEU	2.6
1	B	265	VAL	2.6
1	B	232	GLN	2.6
1	B	485	ALA	2.6
1	B	561	LEU	2.6
1	B	62	ARG	2.6
1	A	516	LEU	2.6
1	B	475	LEU	2.6
1	A	456	ALA	2.5
1	A	589	VAL	2.5
1	B	349	TRP	2.5
1	B	193	GLN	2.5
1	A	127	PHE	2.5
1	A	150	TYR	2.5
1	B	522	ARG	2.5
1	B	295	LEU	2.5
1	A	116	GLN	2.5
1	B	226	GLN	2.5
1	A	633	LEU	2.4
1	A	620	PHE	2.4
1	A	618	LEU	2.4
1	B	115	TYR	2.4
1	B	489	GLN	2.4
1	A	194	ILE	2.4
1	A	636	LEU	2.4
1	B	134	TRP	2.4
1	A	133	GLY	2.3
1	B	273	PHE	2.3
1	A	43	PHE	2.3
1	A	33	ALA	2.3
1	B	438	SER	2.3
1	B	50	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	445	TYR	2.3
1	A	49	PHE	2.2
1	B	467	TRP	2.2
1	A	153	VAL	2.2
1	A	115	TYR	2.2
1	A	485	ALA	2.2
1	A	62	ARG	2.2
1	B	654	ALA	2.2
1	B	604	ASP	2.2
1	B	264	LEU	2.1
1	A	31	VAL	2.1
1	B	116	GLN	2.1
1	B	439	ALA	2.1
1	B	333	PHE	2.1
1	A	255	ARG	2.1
1	A	166	ILE	2.1
1	A	32	GLU	2.1
1	A	556	ALA	2.1
1	B	127	PHE	2.1
1	A	189	SER	2.1
1	B	498	TYR	2.1
1	A	110	VAL	2.1
1	A	467	TRP	2.1
1	A	574	TYR	2.1
1	B	465	TYR	2.0
1	A	126	THR	2.0
1	B	20	THR	2.0
1	B	337	ALA	2.0
1	B	157	LEU	2.0
1	A	581	SER	2.0
1	B	268	GLY	2.0
1	A	576	LEU	2.0
1	B	523	ASP	2.0
1	B	559	LYS	2.0
1	B	625	LYS	2.0
1	A	475	LEU	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, 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	ZN	B	1001	1/1	0.97	0.16	-0.90	96,96,96,96	1
2	ZN	A	1001	1/1	0.88	0.13	-1.16	90,90,90,90	1
2	ZN	A	1002	1/1	0.99	0.06	-3.61	106,106,106,106	1
2	ZN	B	1002	1/1	0.99	0.04	-4.39	102,102,102,102	1

6.5 Other polymers (i)

There are no such residues in this entry.