Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:17 AM GMT

PDB ID	:	2CKG
Title	:	THE STRUCTURE OF SENP1 SUMO-2 CO-COMPLEX SUGGESTS A STRUCTURAL BASIS FOR DISCRIMINATION BETWEEN SUMO PARALOGUES DURING PROCESSING
Authors	:	Dong, C.; Naismith, J.H.
Deposited on	:	2006-04-18
Resolution	:	2.45 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 (i) symbol.

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

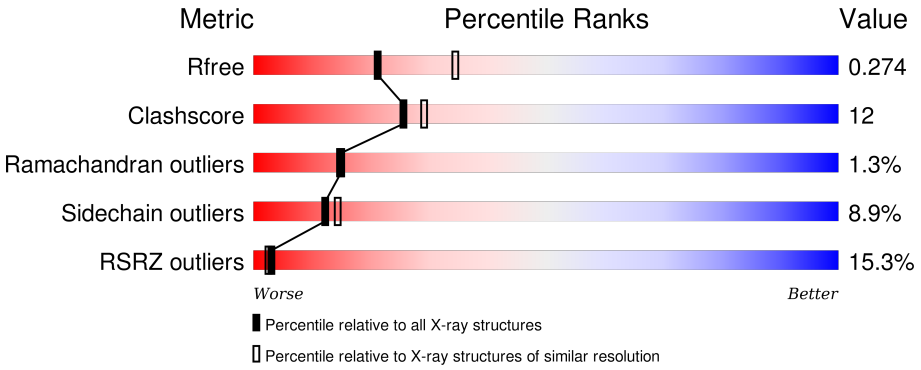
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.45 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	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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	225	9% 76% 18% 6%
1	B	225	22% 66% 29% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3840 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 SENTRIN-SPECIFIC PROTEASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1882	1208	326	334	14			
1	B	225	Total	C	N	O	S	0	0	0
			1882	1208	326	334	14			

- Molecule 2 is water.

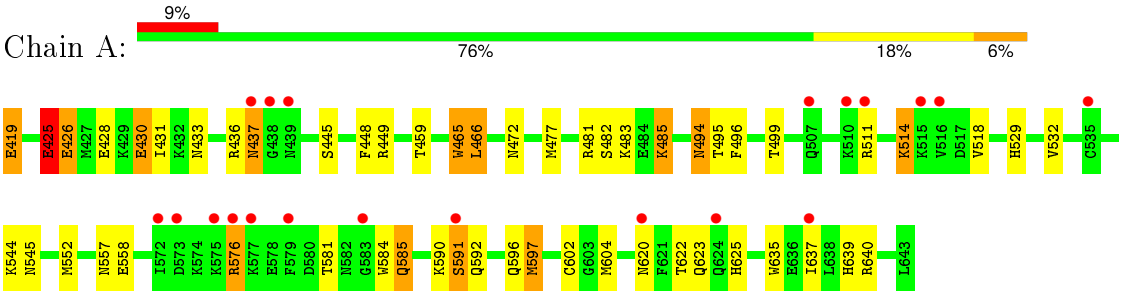
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	44	Total	O	0	0
			44	44		
2	B	32	Total	O	0	0
			32	32		

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.

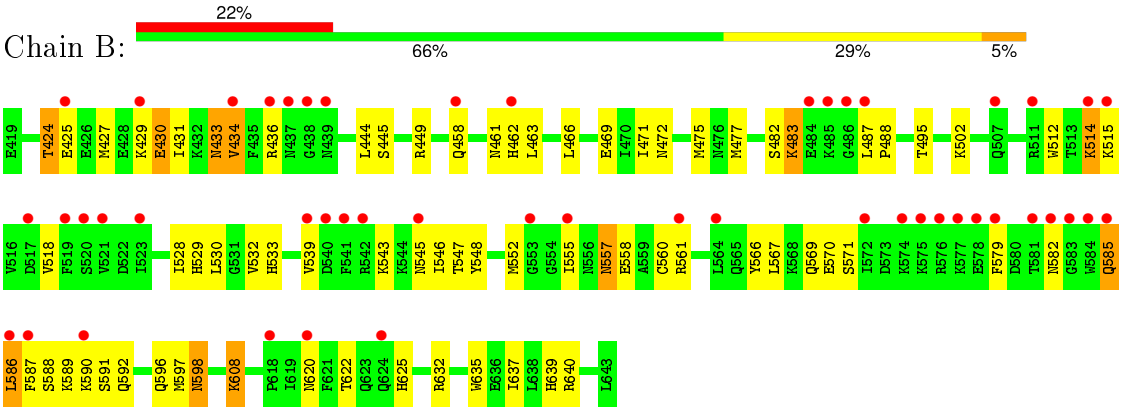
- Molecule 1: SENTRIN-SPECIFIC PROTEASE 1

Chain A:



- Molecule 1: SENTRIN-SPECIFIC PROTEASE 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	71.98Å 71.98Å 200.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	66.96 – 2.45 52.95 – 2.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (66.96-2.45) 100.0 (52.95-2.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.212 , 0.271 0.213 , 0.274	Depositor DCC
R_{free} test set	1136 reflections (5.20%)	DCC
Wilson B-factor (Å^2)	51.4	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 76.2	EDS
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 22968 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3840	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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

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	0.76	3/1925 (0.2%)	0.82	3/2587 (0.1%)
1	B	0.87	7/1925 (0.4%)	0.94	5/2587 (0.2%)
All	All	0.81	10/3850 (0.3%)	0.88	8/5174 (0.2%)

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	1
1	B	0	3
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	585	GLN	CD-NE2	13.53	1.66	1.32
1	B	430	GLU	CB-CG	10.06	1.71	1.52
1	B	585	GLN	CD-OE1	10.00	1.46	1.24
1	A	430	GLU	CB-CG	8.91	1.69	1.52
1	B	561	ARG	CZ-NH1	8.56	1.44	1.33
1	B	561	ARG	NE-CZ	7.92	1.43	1.33
1	B	425	GLU	CG-CD	7.44	1.63	1.51
1	A	430	GLU	CD-OE2	6.84	1.33	1.25
1	B	430	GLU	CD-OE1	6.56	1.32	1.25
1	A	430	GLU	CG-CD	5.16	1.59	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	561	ARG	NE-CZ-NH1	19.86	130.23	120.30
1	B	561	ARG	NE-CZ-NH2	-17.41	111.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	430	GLU	CA-CB-CG	7.01	128.82	113.40
1	A	425	GLU	N-CA-C	5.99	127.18	111.00
1	A	425	GLU	C-N-CA	5.43	135.28	121.70
1	B	430	GLU	CG-CD-OE1	5.27	128.84	118.30
1	B	632	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	430	GLU	CG-CD-OE2	5.15	128.60	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	425	GLU	Peptide
1	B	461	ASN	Peptide
1	B	585	GLN	Sidechain
1	B	596	GLN	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1882	0	1884	44	2
1	B	1882	0	1884	53	2
2	A	44	0	0	8	0
2	B	32	0	0	9	1
All	All	3840	0	3768	94	3

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 12.

All (94) 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:A:482:SER:O	1:A:483:LYS:HB3	1.53	1.03
1:A:576:ARG:HH11	1:A:576:ARG:HG3	1.20	1.02
1:B:430:GLU:OE1	1:B:639:HIS:NE2	1.94	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:GLN:HA	2:A:2028:HOH:O	1.66	0.94
1:B:557:ASN:H	1:B:557:ASN:HD22	1.05	0.94
1:B:482:SER:O	1:B:483:LYS:CB	2.17	0.90
1:B:557:ASN:N	1:B:557:ASN:HD22	1.69	0.90
1:B:462:HIS:HA	2:B:2008:HOH:O	1.70	0.90
1:A:622:THR:H	1:A:625:HIS:HD2	1.23	0.85
1:B:622:THR:H	1:B:625:HIS:HD2	1.26	0.84
1:B:424:THR:HG22	1:B:427:MET:HG3	1.63	0.81
1:B:429:LYS:HE3	2:B:2005:HOH:O	1.78	0.81
1:A:448:PHE:O	1:A:449:ARG:HB2	1.82	0.80
1:A:576:ARG:NH1	1:A:576:ARG:HG3	1.95	0.79
1:B:482:SER:O	1:B:483:LYS:HB2	1.83	0.76
1:B:557:ASN:H	1:B:557:ASN:ND2	1.81	0.76
1:A:511:ARG:O	1:A:514:LYS:HG2	1.87	0.75
1:A:622:THR:H	1:A:625:HIS:CD2	2.04	0.74
1:A:430:GLU:OE2	1:A:639:HIS:NE2	2.24	0.71
1:A:437:ASN:H	1:A:437:ASN:ND2	1.88	0.71
1:A:482:SER:O	1:A:483:LYS:CB	2.29	0.71
1:B:482:SER:O	1:B:483:LYS:HB3	1.91	0.68
1:A:465:TRP:HZ3	1:B:558:GLU:HG2	1.60	0.66
1:A:449:ARG:HG3	1:A:449:ARG:HH11	1.60	0.66
1:B:622:THR:H	1:B:625:HIS:CD2	2.11	0.65
1:B:558:GLU:HB3	2:B:2020:HOH:O	1.96	0.65
1:B:458:GLN:HB2	2:B:2007:HOH:O	1.97	0.63
1:B:424:THR:HG22	1:B:427:MET:CG	2.29	0.62
1:B:539:VAL:HG22	1:B:546:ILE:HG12	1.81	0.61
1:A:485:LYS:NZ	2:A:2014:HOH:O	2.33	0.61
1:A:483:LYS:HA	2:A:2012:HOH:O	2.00	0.60
1:A:576:ARG:HH11	1:A:576:ARG:CG	2.06	0.59
1:B:462:HIS:CG	1:B:463:LEU:H	2.15	0.59
1:B:557:ASN:HB3	2:B:2023:HOH:O	2.03	0.58
1:A:477:MET:CE	1:A:637:ILE:HG12	2.34	0.57
1:A:544:LYS:O	1:A:584:TRP:HA	2.05	0.57
1:B:557:ASN:ND2	1:B:557:ASN:N	2.42	0.56
1:B:462:HIS:CA	2:B:2008:HOH:O	2.41	0.56
1:A:477:MET:HE2	1:A:637:ILE:HG12	1.86	0.55
1:B:514:LYS:O	1:B:515:LYS:HB2	2.07	0.55
1:A:494:ASN:HB2	2:A:2008:HOH:O	2.06	0.54
1:A:597:MET:HB2	1:A:623:GLN:HG2	1.89	0.54
1:B:477:MET:HE1	1:B:637:ILE:HG12	1.90	0.53
1:A:433:ASN:HA	1:A:436:ARG:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:MET:HE1	1:B:530:LEU:HB3	1.92	0.52
1:B:472:ASN:OD1	1:B:495:THR:HG23	2.10	0.51
1:B:548:TYR:HB3	1:B:588:SER:HA	1.91	0.51
1:B:482:SER:HB2	1:B:488:PRO:O	2.10	0.51
1:B:566:TYR:HA	1:B:569:GLN:HE21	1.75	0.51
1:B:429:LYS:NZ	2:B:2004:HOH:O	2.44	0.50
1:A:465:TRP:CZ3	1:B:558:GLU:HG2	2.44	0.50
1:B:560:CYS:HB3	1:B:586:LEU:HB3	1.94	0.49
1:B:571:SER:CB	1:B:579:PHE:HB2	2.43	0.48
1:A:591:SER:O	2:A:2028:HOH:O	2.20	0.48
1:A:448:PHE:O	1:A:449:ARG:CB	2.60	0.48
1:B:430:GLU:HG3	1:B:635:TRP:HE1	1.79	0.47
1:B:512:TRP:CD1	1:B:512:TRP:N	2.83	0.47
1:A:590:LYS:O	1:A:592:GLN:N	2.39	0.46
1:B:543:LYS:HB3	1:B:545:ASN:ND2	2.31	0.46
1:A:596:GLN:HE22	1:A:602:CYS:HB3	1.81	0.46
1:A:545:ASN:HB2	1:A:585:GLN:O	2.16	0.46
1:B:590:LYS:O	1:B:592:GLN:N	2.44	0.46
1:B:608:LYS:HD2	1:B:608:LYS:HA	1.75	0.45
1:B:434:VAL:CG2	1:B:444:LEU:HD13	2.47	0.45
1:B:469:GLU:HG2	2:B:2011:HOH:O	2.16	0.45
1:A:419:GLU:HG2	2:A:2001:HOH:O	2.15	0.45
1:B:431:ILE:HD11	1:B:635:TRP:HB2	1.99	0.44
1:A:494:ASN:HD21	1:A:496:PHE:HD1	1.65	0.44
1:B:532:VAL:O	2:B:2018:HOH:O	2.21	0.44
1:B:597:MET:O	1:B:598:ASN:HB2	2.17	0.44
1:A:431:ILE:HD11	1:A:635:TRP:HB2	1.99	0.44
1:A:433:ASN:O	1:A:436:ARG:HB2	2.17	0.44
1:B:590:LYS:C	1:B:592:GLN:H	2.21	0.43
1:A:485:LYS:HD2	1:A:485:LYS:HA	1.65	0.43
1:B:543:LYS:HB3	1:B:545:ASN:HD21	1.83	0.43
1:A:483:LYS:HB2	2:A:2011:HOH:O	2.18	0.43
1:A:449:ARG:NH1	1:A:449:ARG:HG3	2.28	0.43
1:A:459:THR:HB	1:A:465:TRP:O	2.19	0.42
1:B:424:THR:HG22	1:B:427:MET:H	1.85	0.42
1:B:433:ASN:O	1:B:436:ARG:HG3	2.20	0.41
1:B:462:HIS:CG	1:B:463:LEU:N	2.83	0.41
1:B:533:HIS:CE1	1:B:552:MET:HG3	2.55	0.41
1:B:589:LYS:HD2	1:B:589:LYS:HA	1.78	0.41
1:A:581:THR:O	1:A:584:TRP:HB2	2.21	0.41
1:A:481:ARG:C	1:A:482:SER:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:GLU:N	1:A:426:GLU:HB2	2.36	0.41
1:A:425:GLU:O	1:A:428:GLU:HB2	2.20	0.41
1:B:518:VAL:HG11	1:B:570:GLU:HG2	2.01	0.41
1:B:539:VAL:HG11	1:B:567:LEU:HD11	2.03	0.41
1:B:471:ILE:O	1:B:475:MET:HG2	2.21	0.41
1:B:430:GLU:OE1	1:B:639:HIS:CE1	2.71	0.40
1:A:640:ARG:HD3	2:A:2041:HOH:O	2.20	0.40
1:A:472:ASN:OD1	1:A:495:THR:HG23	2.22	0.40
1:A:466:LEU:HD21	1:A:604:MET:HG2	2.04	0.40

All (3) 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:430:GLU:OE2	1:B:430:GLU:OE1[3_654]	1.26	0.94
1:A:639:HIS:NE2	1:B:430:GLU:OE1[3_654]	2.03	0.17
2:B:2004:HOH:O	2:B:2009:HOH:O[6_555]	2.13	0.07

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	223/225 (99%)	207 (93%)	13 (6%)	3 (1%)	15	15
1	B	223/225 (99%)	207 (93%)	13 (6%)	3 (1%)	15	15
All	All	446/450 (99%)	414 (93%)	26 (6%)	6 (1%)	15	15

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	591	SER
1	B	483	LYS

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Mol	Chain	Res	Type
1	A	426	GLU
1	B	591	SER
1	A	557	ASN
1	B	598	ASN

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	208/208 (100%)	191 (92%)	17 (8%)	14 18
1	B	208/208 (100%)	188 (90%)	20 (10%)	10 12
All	All	416/416 (100%)	379 (91%)	37 (9%)	12 14

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	419	GLU
1	A	437	ASN
1	A	445	SER
1	A	465	TRP
1	A	466	LEU
1	A	485	LYS
1	A	494	ASN
1	A	499	THR
1	A	514	LYS
1	A	518	VAL
1	A	529	HIS
1	A	532	VAL
1	A	558	GLU
1	A	576	ARG
1	A	585	GLN
1	A	597	MET
1	A	620	ASN
1	B	424	THR
1	B	433	ASN

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Mol	Chain	Res	Type
1	B	434	VAL
1	B	445	SER
1	B	449	ARG
1	B	466	LEU
1	B	487	LEU
1	B	502	LYS
1	B	514	LYS
1	B	528	ILE
1	B	529	HIS
1	B	547	THR
1	B	555	ILE
1	B	557	ASN
1	B	582	ASN
1	B	586	LEU
1	B	587	PHE
1	B	608	LYS
1	B	620	ASN
1	B	640	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	437	ASN
1	A	440	GLN
1	A	569	GLN
1	A	582	ASN
1	A	596	GLN
1	A	625	HIS
1	B	545	ASN
1	B	557	ASN
1	B	569	GLN
1	B	582	ASN
1	B	625	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

There are no ligands in this entry.

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	225/225 (100%)	0.92	20 (8%) 12 12	57, 66, 77, 86	0
1	B	225/225 (100%)	1.38	49 (21%) 1 1	55, 66, 77, 83	0
All	All	450/450 (100%)	1.15	69 (15%) 3 2	55, 66, 77, 86	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	437	ASN	9.6
1	A	576	ARG	7.9
1	B	582	ASN	6.3
1	B	541	PHE	6.0
1	B	579	PHE	5.9
1	B	583	GLY	5.5
1	B	620	ASN	5.4
1	B	436	ARG	5.3
1	A	511	ARG	5.2
1	B	521	VAL	4.3
1	B	542	ARG	4.2
1	A	437	ASN	4.2
1	B	618	PRO	4.0
1	B	586	LEU	4.0
1	A	583	GLY	4.0
1	B	576	ARG	3.9
1	B	584	TRP	3.9
1	B	462	HIS	3.8
1	B	434	VAL	3.8
1	B	555	ILE	3.7
1	B	438	GLY	3.7
1	B	587	PHE	3.6
1	B	540	ASP	3.6
1	B	575	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	519	PHE	3.4
1	B	511	ARG	3.4
1	A	515	LYS	3.3
1	B	523	ILE	3.3
1	A	577	LYS	3.2
1	B	425	GLU	3.2
1	B	517	ASP	3.2
1	A	439	ASN	3.2
1	B	545	ASN	3.1
1	A	575	LYS	3.1
1	B	572	ILE	3.0
1	A	516	VAL	2.9
1	B	585	GLN	2.9
1	B	577	LYS	2.9
1	B	439	ASN	2.9
1	B	458	GLN	2.9
1	B	515	LYS	2.8
1	A	572	ILE	2.7
1	B	578	GLU	2.7
1	B	539	VAL	2.7
1	A	624	GLN	2.7
1	B	581	THR	2.7
1	B	564	LEU	2.6
1	B	485	LYS	2.6
1	B	520	SER	2.5
1	A	507	GLN	2.5
1	A	591	SER	2.5
1	B	624	GLN	2.4
1	A	535	CYS	2.4
1	B	486	GLY	2.3
1	B	507	GLN	2.3
1	B	590	LYS	2.3
1	B	561	ARG	2.3
1	B	429	LYS	2.3
1	A	510	LYS	2.2
1	B	574	LYS	2.2
1	A	637	ILE	2.2
1	B	553	GLY	2.2
1	A	438	GLY	2.2
1	B	484	GLU	2.1
1	A	573	ASP	2.1
1	B	514	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	620	ASN	2.1
1	A	579	PHE	2.0
1	B	487	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.