Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:37 PM GMT

PDB ID	:	4YHC
Title	:	Crystal structure of the WD40 domain of SCAP from fission yeast
Authors	:	Gong, X.; Li, J.X.; Wu, J.P.; Yan, C.Y.; Yan, N.
Deposited on	:	2015-02-27
Resolution	:	2.05 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:

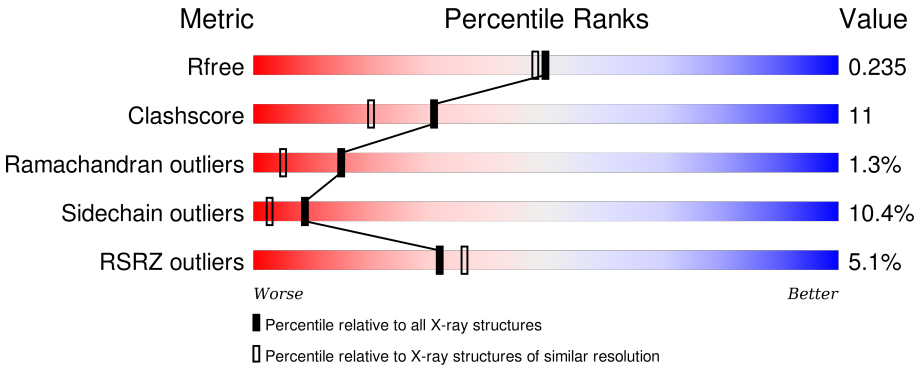
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.05 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	468	3% 75% 15% • 6%
1	B	468	7% 61% 22% • 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7087 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 Sterol regulatory element-binding protein cleavage-activating protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	1	0
			3486	2227	571	676	12			
1	B	411	Total	C	N	O	S	0	0	0
			3268	2099	532	625	12			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	566	MET	-	expression tag	UNP O43043
A	618	SER	CYS	engineered mutation	UNP O43043
A	671	SER	CYS	engineered mutation	UNP O43043
A	680	SER	CYS	engineered mutation	UNP O43043
A	756	SER	CYS	engineered mutation	UNP O43043
A	873	SER	CYS	engineered mutation	UNP O43043
A	901	SER	CYS	engineered mutation	UNP O43043
A	920	SER	CYS	engineered mutation	UNP O43043
A	941	SER	CYS	engineered mutation	UNP O43043
A	983	ALA	-	linker	UNP O43043
A	984	GLY	-	linker	UNP O43043
A	985	SER	-	linker	UNP O43043
A	1010	SER	CYS	engineered mutation	UNP O43043
B	566	MET	-	expression tag	UNP O43043
B	618	SER	CYS	engineered mutation	UNP O43043
B	671	SER	CYS	engineered mutation	UNP O43043
B	680	SER	CYS	engineered mutation	UNP O43043
B	756	SER	CYS	engineered mutation	UNP O43043
B	873	SER	CYS	engineered mutation	UNP O43043
B	901	SER	CYS	engineered mutation	UNP O43043
B	920	SER	CYS	engineered mutation	UNP O43043
B	941	SER	CYS	engineered mutation	UNP O43043
B	983	ALA	-	linker	UNP O43043
B	984	GLY	-	linker	UNP O43043

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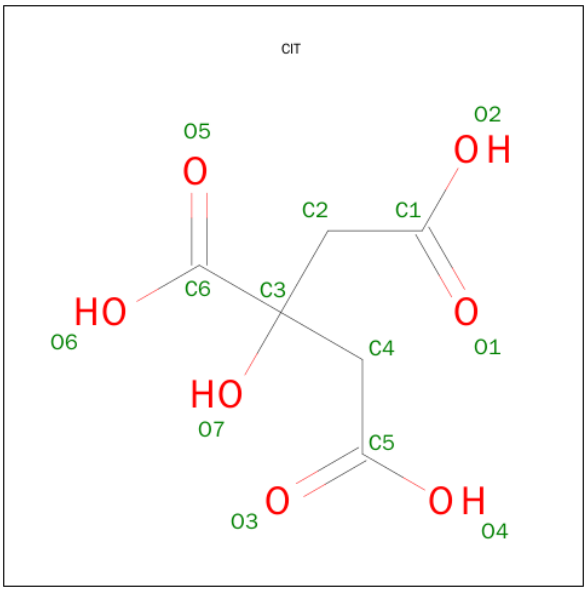
Chain	Residue	Modelled	Actual	Comment	Reference
B	985	SER	-	linker	UNP O43043
B	1010	SER	CYS	engineered mutation	UNP O43043

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 6 7	0	0
2	A	1	Total C O 13 6 7	0	0

- Molecule 3 is water.

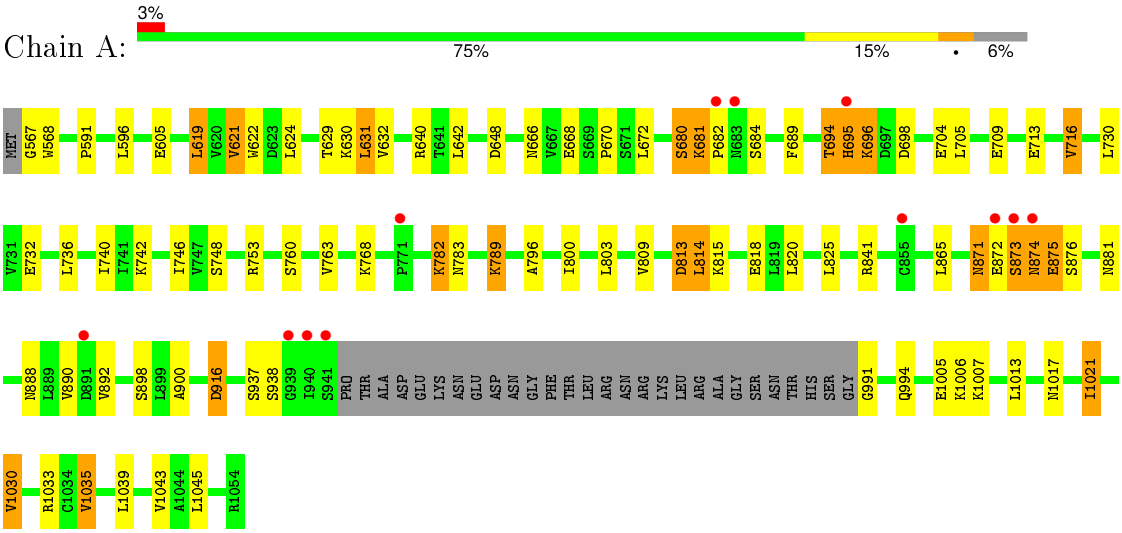
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	204	Total O 204 204	0	0
3	B	103	Total O 103 103	0	0

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.

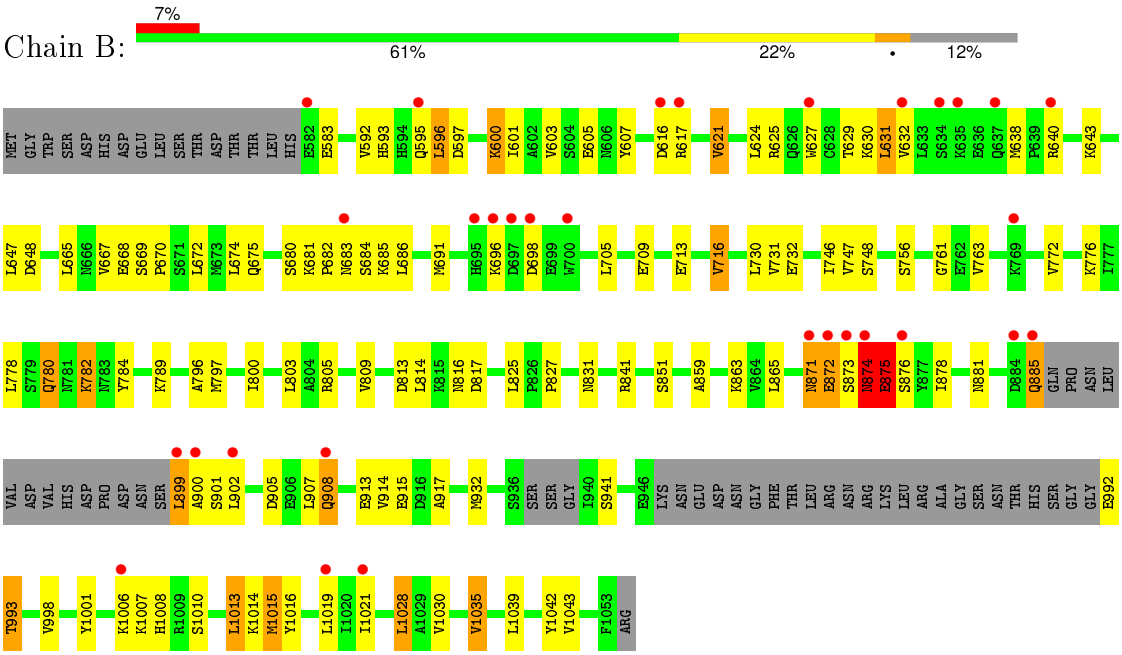
- Molecule 1: Sterol regulatory element-binding protein cleavage-activating protein

Chain A:



- Molecule 1: Sterol regulatory element-binding protein cleavage-activating protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	38.01Å 109.71Å 103.45Å 90.00° 100.46° 90.00°	Depositor
Resolution (Å)	40.00 – 2.05 46.15 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.2 (40.00-2.05) 99.2 (46.15-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.06 (at 2.05Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.177 , 0.229 0.182 , 0.235	Depositor DCC
R_{free} test set	2658 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	29.3	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 59.0	EDS
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 52033 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7087	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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: CIT

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	0.90	0/3565	0.96	12/4840 (0.2%)
1	B	0.79	0/3339	0.89	4/4525 (0.1%)
All	All	0.85	0/6904	0.92	16/9365 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1035	VAL	CG1-CB-CG2	8.85	125.07	110.90
1	A	1030	VAL	CG1-CB-CG2	6.78	121.75	110.90
1	B	1035	VAL	CG1-CB-CG2	6.75	121.69	110.90
1	A	1033	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	A	1033	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	B	941	SER	C-N-CD	5.84	140.67	128.40
1	A	813	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	B	1028	LEU	CA-CB-CG	5.56	128.09	115.30
1	A	619	LEU	CA-CB-CG	5.45	127.84	115.30
1	A	1035	VAL	CA-CB-CG1	5.42	119.04	110.90
1	A	814	LEU	CA-CB-CG	5.31	127.52	115.30
1	A	689	PHE	CB-CA-C	-5.26	99.89	110.40
1	A	813	ASP	CB-CG-OD1	5.25	123.02	118.30
1	A	619	LEU	CB-CG-CD2	5.24	119.91	111.00
1	A	865	LEU	CA-CB-CG	5.14	127.11	115.30
1	B	805	ARG	NE-CZ-NH1	-5.10	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3486	0	3421	55	0
1	B	3268	0	3245	91	0
2	A	26	0	10	2	0
3	A	204	0	0	5	0
3	B	103	0	0	4	0
All	All	7087	0	6676	147	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 11.

All (147) 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:876:SER:HB3	1:B:902:LEU:CD1	1.54	1.34
1:B:876:SER:CB	1:B:902:LEU:HD11	1.59	1.29
1:B:1014:LYS:HE3	1:B:1016:TYR:OH	1.48	1.12
1:B:876:SER:HB3	1:B:902:LEU:HD11	1.11	1.08
1:B:871:ASN:H	1:B:872:GLU:HB2	1.19	1.06
1:A:682:PRO:HA	1:A:684:SER:H	1.36	0.89
1:A:809:VAL:HG23	1:A:825:LEU:HD12	1.54	0.89
1:B:871:ASN:H	1:B:872:GLU:CB	1.88	0.85
1:B:998:VAL:HG23	1:B:1013:LEU:HD21	1.60	0.84
1:B:873:SER:C	1:B:874:ASN:OD1	2.16	0.83
1:B:871:ASN:ND2	1:B:875:GLU:OE2	2.15	0.80
1:B:800:ILE:HD11	1:B:881:ASN:HB2	1.63	0.79
1:A:736:LEU:HD22	1:A:740:ILE:HD11	1.67	0.77
1:B:851:SER:HB3	1:B:872:GLU:HG3	1.69	0.74
1:B:998:VAL:CG2	1:B:1013:LEU:HD21	2.19	0.73
1:A:888:ASN:OD1	1:A:890:VAL:HG23	1.88	0.73
1:B:932:MET:HG2	1:B:998:VAL:HG22	1.72	0.72
1:B:643:LYS:NZ	1:B:684:SER:O	2.23	0.72
1:B:871:ASN:N	1:B:872:GLU:HB2	2.01	0.72
1:B:998:VAL:HG23	1:B:1013:LEU:CD2	2.21	0.71
1:B:876:SER:HB3	1:B:902:LEU:HD13	1.69	0.69
1:B:1008:HIS:CE1	3:B:1158:HOH:O	2.44	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:LYS:HG2	1:A:709:GLU:OE1	1.93	0.68
1:B:873:SER:O	1:B:875:GLU:N	2.27	0.68
1:B:809:VAL:HG23	1:B:825:LEU:HD12	1.77	0.66
1:A:815:LYS:O	3:A:1401:HOH:O	2.13	0.66
1:A:872:GLU:CD	1:A:873:SER:H	1.99	0.66
1:A:682:PRO:HA	1:A:684:SER:N	2.11	0.65
1:A:782:LYS:H	1:A:782:LYS:HE2	1.61	0.65
1:B:1014:LYS:HE3	1:B:1016:TYR:CZ	2.32	0.65
1:A:783:ASN:ND2	3:A:1201:HOH:O	2.19	0.65
1:B:876:SER:HB2	1:B:902:LEU:HD11	1.72	0.64
1:B:871:ASN:H	1:B:872:GLU:CA	2.11	0.63
1:B:789:LYS:HG2	1:B:803:LEU:HD21	1.83	0.61
1:B:583:GLU:HG2	1:B:583:GLU:O	2.02	0.60
1:A:873:SER:O	1:A:875:GLU:N	2.35	0.59
1:B:876:SER:CB	1:B:902:LEU:CD1	2.36	0.59
1:A:680:SER:O	1:A:682:PRO:HD2	2.03	0.58
1:A:871:ASN:O	1:A:872:GLU:HB3	2.03	0.57
1:A:1021:ILE:H	1:A:1021:ILE:HD13	1.70	0.57
1:A:1021:ILE:N	1:A:1021:ILE:HD13	2.20	0.57
1:A:630:LYS:NZ	1:A:668:GLU:OE1	2.39	0.56
1:B:1014:LYS:HE3	1:B:1016:TYR:HH	1.65	0.56
1:B:680:SER:HB3	1:B:682:PRO:HD3	1.88	0.55
1:A:782:LYS:H	1:A:782:LYS:CE	2.19	0.55
1:A:872:GLU:HA	1:A:872:GLU:OE2	2.06	0.55
1:B:797:MET:SD	3:B:1182:HOH:O	2.57	0.55
1:B:597:ASP:OD1	1:B:1021:ILE:HD11	2.08	0.54
1:A:629:THR:CG2	1:A:632:VAL:HG23	2.38	0.54
1:B:874:ASN:OD1	1:B:874:ASN:N	2.39	0.54
1:A:629:THR:HG21	1:A:632:VAL:HG23	1.89	0.54
1:B:593:HIS:HB3	1:B:1042:TYR:HB3	1.88	0.54
1:B:647:LEU:HD12	1:B:647:LEU:N	2.23	0.54
1:A:1013:LEU:HD23	1:A:1013:LEU:C	2.28	0.53
1:A:888:ASN:CG	1:A:890:VAL:HG23	2.29	0.53
1:B:607:TYR:CD1	1:B:1030:VAL:O	2.62	0.53
1:A:716:VAL:HG13	1:A:732:GLU:HB2	1.91	0.53
1:B:992:GLU:N	1:B:1019:LEU:HD21	2.24	0.53
1:B:682:PRO:HA	1:B:683:ASN:C	2.29	0.52
1:A:704:GLU:OE2	1:A:768:LYS:HE2	2.10	0.52
1:A:782:LYS:CD	1:A:782:LYS:H	2.21	0.52
1:A:872:GLU:CG	1:A:873:SER:N	2.73	0.52
1:B:685:LYS:NZ	3:B:1103:HOH:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:VAL:HG21	1:B:1030:VAL:HG23	1.92	0.51
1:B:872:GLU:CG	1:B:873:SER:N	2.73	0.51
1:A:666:ASN:O	1:A:670:PRO:HA	2.11	0.51
1:A:916:ASP:HB2	3:A:1387:HOH:O	2.09	0.51
1:B:827:PRO:HB2	1:B:859:ALA:HB3	1.92	0.51
1:B:716:VAL:HG13	1:B:732:GLU:HB2	1.93	0.51
1:B:782:LYS:H	1:B:782:LYS:CE	2.24	0.51
1:B:691:MET:CE	1:B:747:VAL:HG22	2.41	0.51
1:A:695:HIS:O	1:A:696:LYS:CB	2.60	0.50
1:B:592:VAL:HG21	1:B:629:THR:CG2	2.42	0.50
1:B:674:LEU:HD23	1:B:675:GLN:N	2.27	0.49
1:B:876:SER:OG	1:B:902:LEU:HD11	2.10	0.49
1:B:871:ASN:N	1:B:872:GLU:CA	2.73	0.49
1:B:873:SER:O	1:B:874:ASN:OD1	2.30	0.49
1:B:899:LEU:HD12	1:B:899:LEU:C	2.33	0.49
1:B:878:ILE:HG12	1:B:907:LEU:HD21	1.94	0.49
1:A:872:GLU:CG	1:A:873:SER:H	2.25	0.49
1:B:782:LYS:HE2	1:B:782:LYS:H	1.78	0.49
1:B:1016:TYR:O	1:B:1019:LEU:CD1	2.60	0.48
1:B:669:SER:O	1:B:670:PRO:C	2.51	0.48
1:B:993:THR:HA	1:B:1015:MET:O	2.12	0.48
1:B:914:VAL:HG12	1:B:915:GLU:O	2.14	0.48
1:B:681:LYS:HG2	1:B:709:GLU:OE1	2.14	0.48
1:A:800:ILE:HD11	1:A:881:ASN:HB2	1.96	0.48
1:A:680:SER:O	1:A:682:PRO:CD	2.61	0.48
2:A:1102:CIT:O7	2:A:1102:CIT:O2	2.32	0.48
1:A:890:VAL:HG12	1:A:892:VAL:HG13	1.96	0.48
1:B:617:ARG:O	1:B:638:MET:HG3	2.14	0.48
1:A:789:LYS:N	1:A:789:LYS:HD3	2.29	0.47
1:B:680:SER:CB	1:B:682:PRO:HD3	2.44	0.47
1:B:596:LEU:HB2	1:B:616:ASP:HB3	1.97	0.47
1:B:908:GLN:O	1:B:908:GLN:HG3	2.15	0.47
1:A:872:GLU:HG3	1:A:873:SER:N	2.31	0.46
1:B:761:GLY:O	1:B:789:LYS:HD3	2.15	0.46
1:A:742:LYS:NZ	3:A:1337:HOH:O	2.47	0.46
1:A:694:THR:O	1:A:694:THR:OG1	2.26	0.46
1:A:1007:LYS:NZ	3:B:1165:HOH:O	2.48	0.46
1:B:875:GLU:H	1:B:875:GLU:HG3	1.50	0.46
1:B:871:ASN:N	1:B:872:GLU:HA	2.30	0.45
1:B:780:GLN:HG2	1:B:789:LYS:HE2	1.98	0.45
1:A:629:THR:HG21	1:A:632:VAL:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:872:GLU:CD	1:B:873:SER:H	2.19	0.45
1:B:631:LEU:HD23	1:B:632:VAL:N	2.32	0.45
1:B:992:GLU:O	1:B:993:THR:HB	2.16	0.44
1:A:621:VAL:HG13	1:A:631:LEU:HB3	1.99	0.44
1:B:746:ILE:HG23	1:B:796:ALA:HA	1.99	0.44
1:B:665:LEU:HD12	1:B:665:LEU:N	2.32	0.44
1:B:716:VAL:HG22	1:B:731:VAL:HG23	2.00	0.44
1:B:621:VAL:CG2	1:B:630:LYS:HB2	2.48	0.44
1:B:776:LYS:NZ	1:B:817:ASP:OD2	2.51	0.44
1:B:780:GLN:NE2	1:B:784:TYR:O	2.42	0.43
1:B:691:MET:HE3	1:B:747:VAL:HG22	2.00	0.43
1:B:756:SER:O	1:B:763:VAL:HA	2.19	0.43
1:B:813:ASP:O	1:B:817:ASP:HA	2.19	0.43
1:A:746:ILE:HG23	1:A:796:ALA:HA	1.99	0.43
1:A:681:LYS:N	1:A:681:LYS:HD3	2.34	0.43
1:A:1005:GLU:HG2	1:B:772:VAL:HG11	2.00	0.43
1:A:567:GLY:HA2	3:A:1250:HOH:O	2.19	0.43
1:B:816:ASN:ND2	1:B:885:GLN:HG3	2.34	0.43
1:A:809:VAL:CG2	1:A:825:LEU:HD12	2.38	0.43
1:A:680:SER:HB3	1:A:682:PRO:HD3	2.01	0.42
1:B:900:ALA:O	1:B:902:LEU:HD12	2.19	0.42
1:A:873:SER:OG	1:A:874:ASN:N	2.51	0.42
1:A:813:ASP:HB2	1:A:820:LEU:HD11	2.02	0.42
1:A:874:ASN:O	1:A:875:GLU:HG3	2.19	0.42
1:B:600:LYS:HD2	1:B:601:ILE:N	2.35	0.42
1:A:876:SER:HB2	1:A:900:ALA:O	2.20	0.42
1:A:991:GLY:HA3	1:A:1017:ASN:OD1	2.20	0.42
1:B:1001:TYR:CZ	1:B:1006:LYS:HA	2.54	0.42
1:B:685:LYS:N	1:B:685:LYS:HD2	2.35	0.41
1:B:643:LYS:HE3	1:B:686:LEU:HG	2.01	0.41
1:B:681:LYS:O	1:B:682:PRO:C	2.56	0.41
1:B:873:SER:O	1:B:874:ASN:CG	2.59	0.41
1:A:591:PRO:HD2	1:A:622:TRP:CH2	2.55	0.41
1:A:871:ASN:N	1:A:871:ASN:OD1	2.54	0.41
1:A:746:ILE:HB	1:A:753:ARG:HB2	2.03	0.41
1:A:937:SER:HB3	1:A:994:GLN:HG2	2.03	0.41
1:B:1013:LEU:N	1:B:1013:LEU:HD22	2.36	0.41
1:B:601:ILE:HG13	1:B:1028:LEU:HD22	2.01	0.41
1:B:873:SER:C	1:B:874:ASN:CG	2.78	0.41
1:B:863:LYS:HG3	1:B:913:GLU:OE1	2.21	0.40
1:B:597:ASP:OD1	1:B:1021:ILE:CD1	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:915:GLU:HG3	1:B:917:ALA:HB3	2.02	0.40
2:A:1102:CIT:O7	2:A:1102:CIT:O4	2.35	0.40

There are no symmetry-related clashes.

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	436/468 (93%)	418 (96%)	12 (3%)	6 (1%)	14 4
1	B	403/468 (86%)	376 (93%)	22 (6%)	5 (1%)	16 6
All	All	839/936 (90%)	794 (95%)	34 (4%)	11 (1%)	15 5

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	696	LYS
1	A	873	SER
1	A	874	ASN
1	A	875	GLU
1	B	874	ASN
1	B	875	GLU
1	A	898	SER
1	B	696	LYS
1	B	871	ASN
1	B	993	THR
1	A	681	LYS

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	397/424 (94%)	359 (90%)	38 (10%)	10 4
1	B	372/424 (88%)	330 (89%)	42 (11%)	7 2
All	All	769/848 (91%)	689 (90%)	80 (10%)	9 3

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	568	TRP
1	A	596	LEU
1	A	605	GLU
1	A	619	LEU
1	A	621	VAL
1	A	624	LEU
1	A	631	LEU
1	A	640	ARG
1	A	642	LEU
1	A	648	ASP
1	A	672	LEU
1	A	680	SER
1	A	694	THR
1	A	695	HIS
1	A	698	ASP
1	A	705	LEU
1	A	713	GLU
1	A	716	VAL
1	A	730	LEU
1	A	748	SER
1	A	760	SER
1	A	763	VAL
1	A	782	LYS
1	A	789	LYS
1	A	803	LEU
1	A	814	LEU
1	A	818	GLU

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Mol	Chain	Res	Type
1	A	841	ARG
1	A	871	ASN
1	A	916	ASP
1	A	938	SER
1	A	1006	LYS
1	A	1021	ILE
1	A	1030	VAL
1	A	1035	VAL
1	A	1039	LEU
1	A	1043	VAL
1	A	1045	LEU
1	B	595	GLN
1	B	596	LEU
1	B	600	LYS
1	B	605	GLU
1	B	621	VAL
1	B	624	LEU
1	B	625	ARG
1	B	627	TRP
1	B	631	LEU
1	B	640	ARG
1	B	648	ASP
1	B	667	VAL
1	B	668	GLU
1	B	672	LEU
1	B	698	ASP
1	B	705	LEU
1	B	713	GLU
1	B	716	VAL
1	B	730	LEU
1	B	748	SER
1	B	778	LEU
1	B	780	GLN
1	B	782	LYS
1	B	814	LEU
1	B	831	ASN
1	B	841	ARG
1	B	865	LEU
1	B	872	GLU
1	B	874	ASN
1	B	875	GLU
1	B	885	GLN

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Mol	Chain	Res	Type
1	B	899	LEU
1	B	901	SER
1	B	905	ASP
1	B	908	GLN
1	B	1007	LYS
1	B	1010	SER
1	B	1013	LEU
1	B	1015	MET
1	B	1035	VAL
1	B	1039	LEU
1	B	1043	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	581	HIS
1	A	695	HIS
1	B	816	ASN
1	B	1017	ASN

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

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CIT	A	1101	-	3,12,12	1.22	1 (33%)	3,17,17	0.73	0
2	CIT	A	1102	-	3,12,12	1.62	1 (33%)	3,17,17	5.13	3 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	A	1101	-	-	0/6/16/16	0/0/0/0
2	CIT	A	1102	-	-	0/6/16/16	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1102	CIT	C4-C3	-2.44	1.51	1.54
2	A	1101	CIT	C4-C3	-2.08	1.51	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1102	CIT	C3-C2-C1	-7.14	103.55	114.96
2	A	1102	CIT	C3-C4-C5	-4.83	107.23	114.96
2	A	1102	CIT	C4-C3-C2	2.18	115.02	109.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1102	CIT	2	0

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	439/468 (93%)	-0.09	12 (2%)	58	64	16, 30, 69, 129	0
1	B	411/468 (87%)	0.18	31 (7%)	17	20	21, 40, 87, 137	0
All	All	850/936 (90%)	0.04	43 (5%)	32	36	16, 35, 80, 137	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	873	SER	11.2
1	B	873	SER	9.0
1	B	874	ASN	6.5
1	A	941	SER	4.7
1	B	617	ARG	4.3
1	B	900	ALA	4.3
1	B	697	ASP	4.2
1	A	695	HIS	4.1
1	B	899	LEU	4.0
1	B	872	GLU	3.8
1	B	1021	ILE	3.6
1	A	855	CYS	3.6
1	A	872	GLU	3.6
1	B	634	SER	3.6
1	B	885	GLN	3.5
1	B	698	ASP	3.5
1	B	640	ARG	3.4
1	B	637	GLN	3.3
1	B	700	TRP	3.3
1	B	696	LYS	3.3
1	B	769	LYS	3.3
1	A	939	GLY	3.3
1	A	891	ASP	3.1
1	B	902	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	1019	LEU	3.0
1	B	683	ASN	2.7
1	B	627	TRP	2.6
1	B	884	ASP	2.5
1	A	683	ASN	2.5
1	A	874	ASN	2.4
1	B	582	GLU	2.4
1	A	682	PRO	2.4
1	A	940	ILE	2.4
1	B	876	SER	2.4
1	B	632	VAL	2.3
1	B	908	GLN	2.3
1	B	635	LYS	2.2
1	B	595	GLN	2.2
1	A	771	PRO	2.2
1	B	695	HIS	2.2
1	B	616	ASP	2.1
1	B	871	ASN	2.0
1	B	1006	LYS	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	CIT	A	1102	13/13	0.89	0.17	0.62	33,49,67,73	0
2	CIT	A	1101	13/13	0.95	0.10	-0.05	25,35,60,63	0

6.5 Other polymers (i)

There are no such residues in this entry.