



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:04 AM UTC

PDB ID : 4YHC / pdb_00004yhc
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

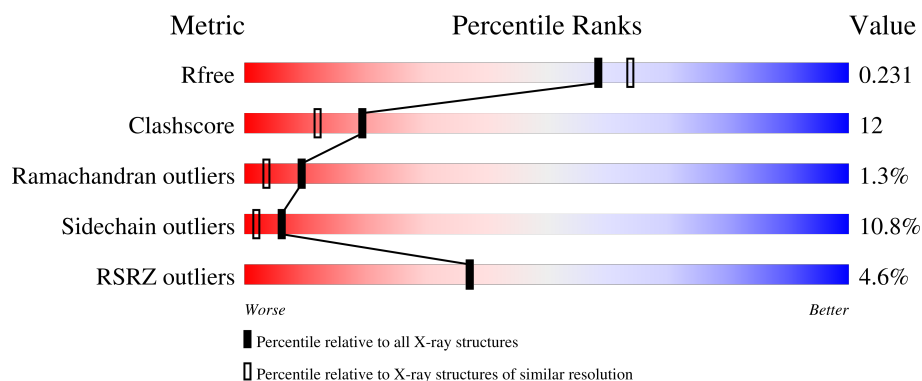
1 Overall quality at a glance

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}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. 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% 73% 17% • 6%
1	B	468	5% 61% 22% 5% 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:

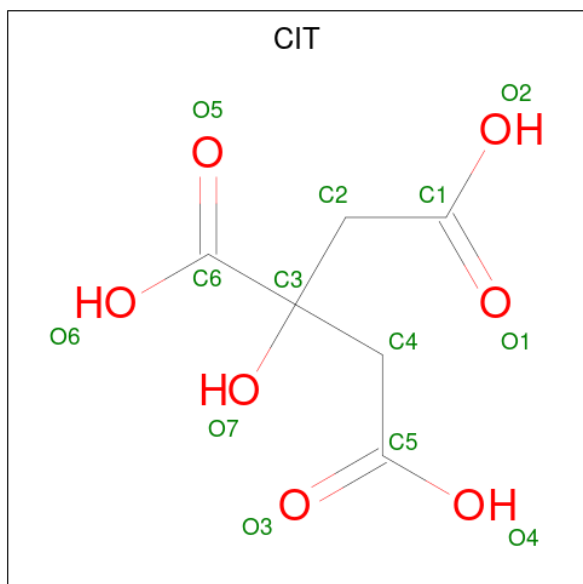
Chain	Residue	Modelled	Actual	Comment	Reference
A	566	MET	-	expression tag	UNP O43043
A	618	SER	CYS	engineered mutation	UNP O43043
A	671	SER	CYS	engineered mutation	UNP O43043
A	680	SER	CYS	engineered mutation	UNP O43043
A	756	SER	CYS	engineered mutation	UNP O43043
A	873	SER	CYS	engineered mutation	UNP 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 (CCD ID: 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

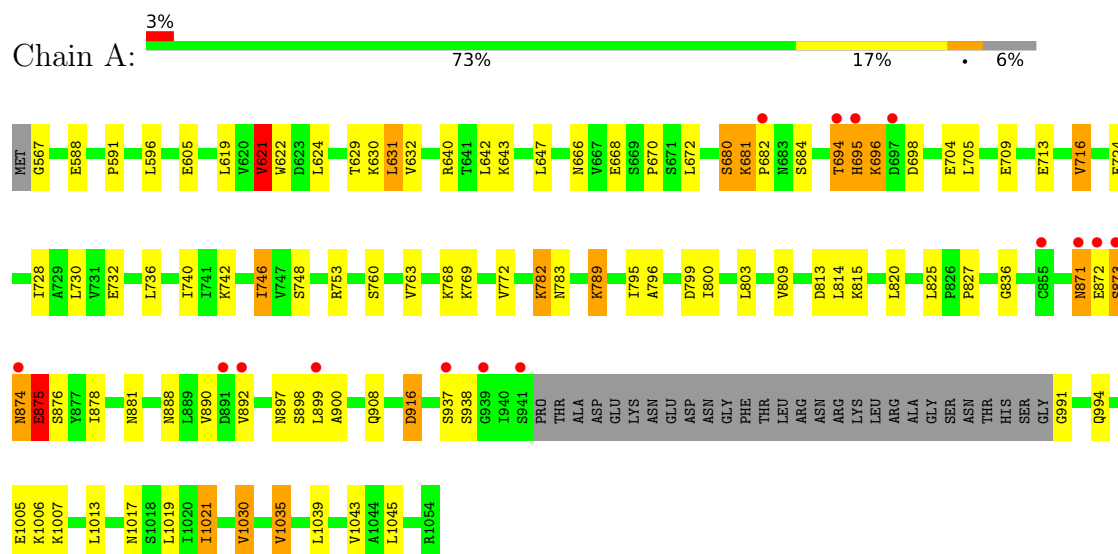
- Molecule 3 is water.

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

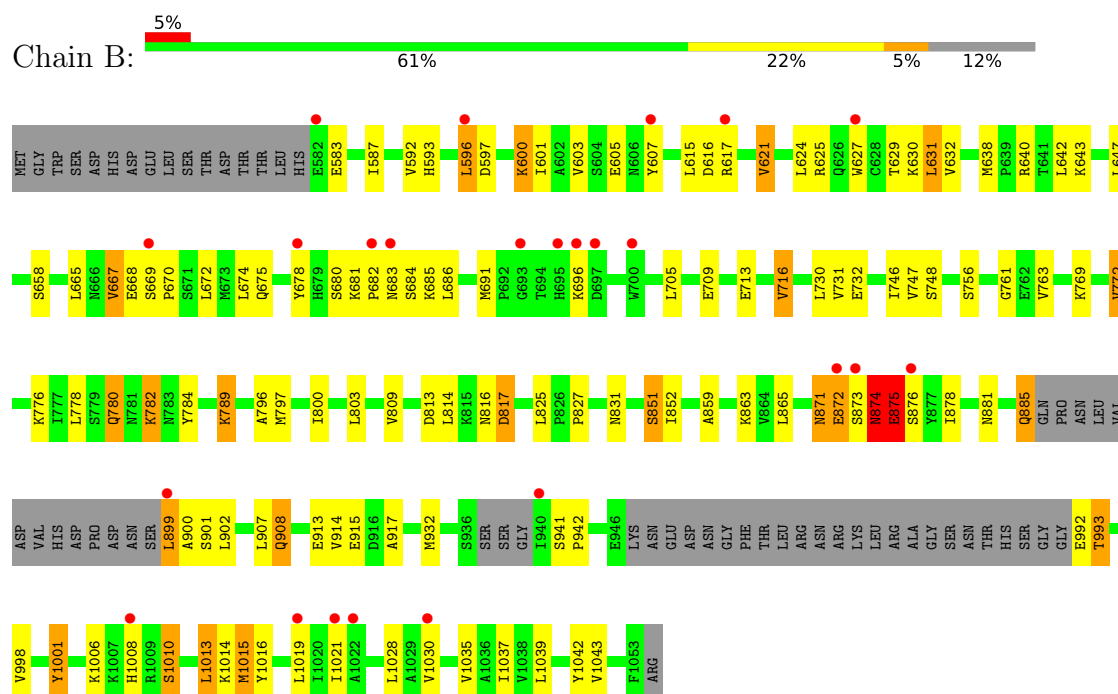
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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



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



4 Data and refinement statistics

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 40.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.2 (40.00-2.05) 99.4 (40.00-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.05Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.177 , 0.229 0.180 , 0.231	Depositor DCC
R_{free} test set	2658 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.21	6/3565 (0.2%)	1.09	9/4840 (0.2%)
1	B	1.04	5/3339 (0.1%)	1.05	5/4525 (0.1%)
All	All	1.13	11/6904 (0.2%)	1.07	14/9365 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1001	TYR	C-O	7.43	1.32	1.23
1	A	728	ILE	C-O	-5.84	1.18	1.23
1	B	1037	ILE	CA-C	5.79	1.60	1.52
1	A	799	ASP	CA-C	5.61	1.60	1.53
1	A	647	LEU	CA-C	-5.50	1.46	1.52
1	A	878	ILE	CA-C	-5.21	1.46	1.52
1	A	827	PRO	N-CA	-5.19	1.40	1.47
1	B	941	SER	C-N	5.13	1.40	1.33
1	B	942	PRO	N-CD	5.04	1.54	1.47
1	A	836	GLY	N-CA	5.03	1.50	1.45
1	B	851	SER	N-CA	5.02	1.51	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1030	VAL	N-CA-CB	-7.97	102.85	112.33
1	A	1030	VAL	CB-CA-C	7.26	118.46	110.62
1	A	1035	VAL	CG1-CB-CG2	6.49	125.07	110.80
1	A	1035	VAL	N-CA-CB	-5.84	101.12	111.93
1	A	772	VAL	N-CA-C	5.82	116.26	108.11
1	B	817	ASP	N-CA-C	5.73	119.30	111.39
1	A	621	VAL	CB-CA-C	5.69	119.31	110.83
1	B	667	VAL	CB-CA-C	5.60	116.98	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	941	SER	CA-C-N	-5.55	113.89	119.56
1	B	941	SER	C-N-CA	-5.55	113.89	119.56
1	B	1010	SER	N-CA-C	5.14	117.06	108.99
1	A	588	GLU	CA-C-N	5.09	124.85	119.76
1	A	588	GLU	C-N-CA	5.09	124.85	119.76
1	A	1035	VAL	CA-CB-CG1	5.08	119.04	110.40

There are no chirality outliers.

There are no planarity outliers.

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	3486	0	3421	59	0
1	B	3268	0	3245	96	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	156	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 12.

All (156) 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:873:SER:C	1:B:874:ASN:OD1	2.16	0.88
1:B:871:ASN:H	1:B:872:GLU:CB	1.88	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:998:VAL:HG23	1:B:1013:LEU:HD21	1.60	0.84
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:A:888:ASN:OD1	1:A:890:VAL:HG23	1.88	0.73
1:B:998:VAL:CG2	1:B:1013:LEU:HD21	2.19	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:691:MET:HE3	1:B:747:VAL:HG22	1.73	0.71
1:B:998:VAL:HG23	1:B:1013:LEU:CD2	2.21	0.71
1:A:872:GLU:CD	1:A:873:SER:H	1.99	0.70
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
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:682:PRO:HA	1:A:684:SER:N	2.11	0.65
1:A:782:LYS:HE2	1:A:782:LYS:H	1.61	0.65
1:A:783:ASN:ND2	3:A:1201:HOH:O	2.19	0.65
1:B:1014:LYS:HE3	1:B:1016:TYR:CZ	2.32	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:O	1:B:583:GLU:HG2	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:888:ASN:CG	1:A:890:VAL:HG23	2.29	0.58
1:A:1013:LEU:C	1:A:1013:LEU:HD23	2.28	0.58
1:A:871:ASN:O	1:A:872:GLU:HB3	2.03	0.57
1:A:1021:ILE:HD13	1:A:1021:ILE:H	1.70	0.57
1:A:1021:ILE:HD13	1:A:1021:ILE:N	2.20	0.57
1:B:1014:LYS:HE3	1:B:1016:TYR:HH	1.64	0.57
1:A:630:LYS:NZ	1:A:668:GLU:OE1	2.39	0.56
1:B:682:PRO:HA	1:B:683:ASN:C	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:899:LEU:C	1:B:899:LEU:HD12	2.33	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:643:LYS:NZ	1:A:684:SER:O	2.33	0.53
1:B:669:SER:O	1:B:670:PRO:C	2.51	0.53
1:A:716:VAL:HG13	1:A:732:GLU:HB2	1.91	0.53
1:B:607:TYR:CD1	1:B:1030:VAL:O	2.62	0.53
1:B:992:GLU:N	1:B:1019:LEU:HD21	2.24	0.53
1:A:704:GLU:OE2	1:A:768:LYS:HE2	2.10	0.52
1:A:782:LYS:H	1:A:782:LYS:CD	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
1:B:603:VAL:HG21	1:B:1030:VAL:HG23	1.92	0.51
1:B:873:SER:C	1:B:874:ASN:CG	2.78	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: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:827:PRO:HB2	1:B:859:ALA:HB3	1.92	0.51
1:A:695:HIS:O	1:A:696:LYS:CB	2.60	0.50
1:B:691:MET:CE	1:B:747:VAL:HG22	2.41	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:871:ASN:N	1:B:872:GLU:CA	2.73	0.49
1:B:876:SER:OG	1:B:902:LEU:HD11	2.10	0.49
1:B:872:GLU:CD	1:B:873:SER:H	2.19	0.49
1:B:873:SER:O	1:B:874:ASN:OD1	2.30	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:H	1:B:782:LYS:HE2	1.78	0.49
1:B:1016:TYR:O	1:B:1019:LEU:CD1	2.60	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:A:800:ILE:HD11	1:A:881:ASN:HB2	1.96	0.48
1:B:681:LYS:HG2	1:B:709:GLU:OE1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:SER:O	1:A:682:PRO:CD	2.61	0.48
2:A:1102:CIT:O2	2:A:1102:CIT:O7	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:B:872:GLU:CD	1:B:873:SER:HG	2.23	0.47
1:A:694:THR:O	1:A:694:THR:OG1	2.26	0.46
1:A:742:LYS:NZ	3:A:1337:HOH:O	2.47	0.46
1:A:872:GLU:HG3	1:A:873:SER:N	2.31	0.46
1:B:681:LYS:O	1:B:682:PRO:C	2.56	0.46
1:B:761:GLY:O	1:B:789:LYS:HD3	2.15	0.46
1:A:1007:LYS:NZ	3:B:1165:HOH:O	2.48	0.46
1:B:873:SER:O	1:B:874:ASN:CG	2.59	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
1:B:631:LEU:HD23	1:B:632:VAL:N	2.32	0.45
1:B:658:SER:O	1:B:678:TYR:OH	2.33	0.45
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:N	1:B:665:LEU:HD12	2.32	0.44
1:B:674:LEU:HD23	1:B:674:LEU:C	2.42	0.44
1:B:716:VAL:HG22	1:B:731:VAL:HG23	2.00	0.44
1:B:992:GLU:O	1:B:993:THR:HB	2.16	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: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:567:GLY:HA2	3:A:1250:HOH:O	2.19	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: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:1013:LEU:C	1:A:1013:LEU:CD2	2.91	0.42
1:A:680:SER:HB3	1:A:682:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873:SER:OG	1:A:874:ASN:N	2.51	0.42
1:A:897:ASN:C	1:A:899:LEU:H	2.27	0.42
1:B:900:ALA:O	1:B:902:LEU:HD12	2.19	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:B:872:GLU:CD	1:B:873:SER:N	2.77	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:A:591:PRO:HD2	1:A:622:TRP:CH2	2.55	0.41
1:A:724:GLU:CD	1:A:724:GLU:H	2.29	0.41
1:A:871:ASN:OD1	1:A:871:ASN:N	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:601:ILE:HG13	1:B:1028:LEU:HD22	2.01	0.41
1:B:1013:LEU:HD22	1:B:1013:LEU:N	2.36	0.41
1:B:691:MET:HE3	1:B:747:VAL:CG2	2.46	0.40
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
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%)	9 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	403/468 (86%)	376 (93%)	22 (6%)	5 (1%)	10	4
All	All	839/936 (90%)	794 (95%)	34 (4%)	11 (1%)	9	3

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 ⓘ

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%)	357 (90%)	40 (10%)	7	3
1	B	372/424 (88%)	329 (88%)	43 (12%)	5	1
All	All	769/848 (91%)	686 (89%)	83 (11%)	6	2

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	596	LEU
1	A	605	GLU
1	A	619	LEU
1	A	621	VAL
1	A	624	LEU

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Mol	Chain	Res	Type
1	A	631	LEU
1	A	640	ARG
1	A	642	LEU
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	746	ILE
1	A	748	SER
1	A	760	SER
1	A	763	VAL
1	A	769	LYS
1	A	782	LYS
1	A	789	LYS
1	A	795	ILE
1	A	803	LEU
1	A	814	LEU
1	A	871	ASN
1	A	875	GLU
1	A	908	GLN
1	A	916	ASP
1	A	938	SER
1	A	1006	LYS
1	A	1019	LEU
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	587	ILE
1	B	596	LEU
1	B	600	LYS
1	B	605	GLU
1	B	615	LEU
1	B	621	VAL
1	B	624	LEU

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Mol	Chain	Res	Type
1	B	625	ARG
1	B	627	TRP
1	B	631	LEU
1	B	640	ARG
1	B	642	LEU
1	B	667	VAL
1	B	668	GLU
1	B	672	LEU
1	B	705	LEU
1	B	713	GLU
1	B	716	VAL
1	B	730	LEU
1	B	748	SER
1	B	769	LYS
1	B	772	VAL
1	B	778	LEU
1	B	780	GLN
1	B	782	LYS
1	B	789	LYS
1	B	814	LEU
1	B	831	ASN
1	B	852	ILE
1	B	865	LEU
1	B	872	GLU
1	B	874	ASN
1	B	875	GLU
1	B	885	GLN
1	B	899	LEU
1	B	901	SER
1	B	908	GLN
1	B	1010	SER
1	B	1013	LEU
1	B	1015	MET
1	B	1035	VAL
1	B	1039	LEU
1	B	1043	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	571	HIS
1	A	581	HIS

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Mol	Chain	Res	Type
1	A	695	HIS
1	A	702	ASN
1	A	844	ASN
1	B	676	HIS
1	B	687	ASN
1	B	816	ASN
1	B	885	GLN
1	B	1017	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	-	12,12,12	1.32	2 (16%)	17,17,17	1.41	4 (23%)
2	CIT	A	1102	-	12,12,12	1.21	1 (8%)	17,17,17	2.28	9 (52%)

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	-	-	4/16/16/16	-
2	CIT	A	1102	-	-	5/16/16/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1102	CIT	C4-C3	-2.38	1.51	1.54
2	A	1101	CIT	O1-C1	2.25	1.29	1.22
2	A	1101	CIT	O4-C5	-2.17	1.23	1.30

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1102	CIT	O6-C6-C3	4.56	121.88	113.14
2	A	1102	CIT	C3-C2-C1	-3.79	103.55	113.92
2	A	1101	CIT	O6-C6-C3	3.20	119.28	113.14
2	A	1102	CIT	O7-C3-C2	-3.14	102.21	109.38
2	A	1102	CIT	O7-C3-C6	2.76	112.87	108.96
2	A	1102	CIT	O1-C1-C2	-2.51	115.84	122.95
2	A	1102	CIT	C3-C4-C5	-2.45	107.23	113.92
2	A	1101	CIT	O4-C5-C4	2.41	121.99	114.35
2	A	1102	CIT	O5-C6-C3	-2.36	117.52	122.09
2	A	1101	CIT	O3-C5-C4	-2.32	116.38	122.95
2	A	1101	CIT	O7-C3-C6	2.31	112.24	108.96
2	A	1102	CIT	C4-C3-C2	2.22	115.02	109.31
2	A	1102	CIT	O2-C1-C2	2.18	121.25	114.35

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1102	CIT	C2-C3-C6-O6
2	A	1101	CIT	C3-C4-C5-O4
2	A	1101	CIT	C3-C4-C5-O3
2	A	1102	CIT	O2-C1-C2-C3
2	A	1102	CIT	O1-C1-C2-C3
2	A	1102	CIT	C3-C4-C5-O3
2	A	1101	CIT	O1-C1-C2-C3
2	A	1101	CIT	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	A	1102	CIT	C3-C4-C5-O4

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 [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	439/468 (93%)	-0.08	15 (3%) 48 48	16, 30, 69, 129	1 (0%)
1	B	411/468 (87%)	0.25	24 (5%) 29 29	21, 40, 87, 137	0
All	All	850/936 (90%)	0.08	39 (4%) 37 37	16, 35, 80, 137	1 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	873	SER	4.7
1	B	940	ILE	4.5
1	B	697	ASP	4.4
1	B	873	SER	4.4
1	A	872	GLU	3.9
1	A	855	CYS	3.7
1	A	682	PRO	3.7
1	A	695	HIS	3.7
1	B	700	TRP	3.5
1	B	872	GLU	3.3
1	A	697	ASP	3.1
1	B	1021	ILE	3.0
1	A	941	SER	2.9
1	A	891	ASP	2.9
1	A	939	GLY	2.9
1	B	695	HIS	2.8
1	B	693	GLY	2.7
1	B	899	LEU	2.7
1	B	627	TRP	2.7
1	A	694	THR	2.6
1	B	1008	HIS	2.6
1	B	669	SER	2.6
1	B	682	PRO	2.6
1	B	876	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	1019	LEU	2.4
1	B	683	ASN	2.4
1	A	892	VAL	2.4
1	A	874	ASN	2.4
1	A	871	ASN	2.3
1	A	937	SER	2.3
1	B	596	LEU	2.3
1	B	678	TYR	2.3
1	B	617	ARG	2.2
1	A	899	LEU	2.2
1	B	607	TYR	2.1
1	B	582	GLU	2.1
1	B	1022	ALA	2.1
1	B	1030	VAL	2.0
1	B	696	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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CIT	A	1102	13/13	0.85	0.10	33,49,67,73	0
2	CIT	A	1101	13/13	0.95	0.07	25,35,60,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.