



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:26 PM UTC

PDB ID : 6BYF / pdb_00006byf
Title : Crystal structure of the core catalytic domain of PP-IP phosphatase SIW14 from *S. cerevisiae* in complex with citrate
Authors : Wang, H.; Shears, S.B.
Deposited on : 2017-12-20
Resolution : 2.35 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

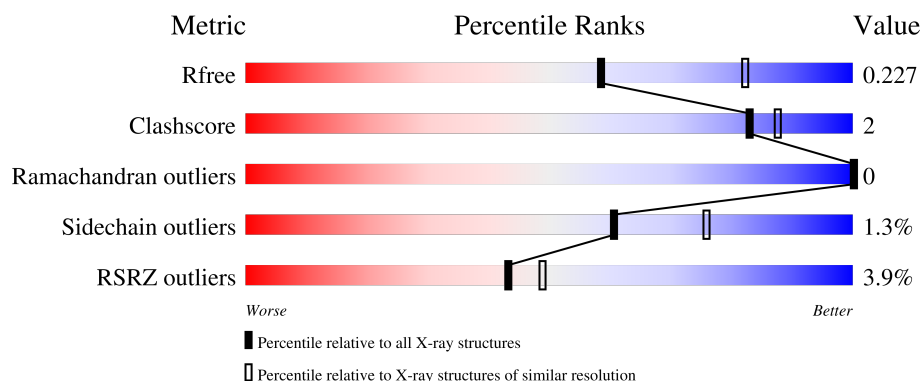
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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 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	170	2% 86% 11% ..
1	B	170	3% 93% ..
1	C	170	% 89% 6% ..
1	D	170	4% 89% 8% ..
1	E	170	4% 90% 6% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	170	5% 88% 7% 5%
1	G	170	6% 95%
1	H	170	5% 86% 9%
1	I	170	4% 89% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12692 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 Tyrosine-protein phosphatase SIW14.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	Se	0	0	0
			1355	874	238	237	3	3			
1	B	164	Total	C	N	O	S	Se	0	0	0
			1356	878	237	235	3	3			
1	C	163	Total	C	N	O	S	Se	0	0	0
			1345	869	236	234	3	3			
1	D	165	Total	C	N	O	S	Se	0	0	0
			1355	874	238	237	3	3			
1	E	164	Total	C	N	O	S	Se	0	0	0
			1356	878	237	235	3	3			
1	F	162	Total	C	N	O	S	Se	0	1	0
			1345	870	235	233	3	4			
1	G	164	Total	C	N	O	S	Se	0	0	0
			1347	870	236	235	3	3			
1	H	163	Total	C	N	O	S	Se	0	0	0
			1345	869	236	234	3	3			
1	I	163	Total	C	N	O	S	Se	0	0	0
			1345	869	236	234	3	3			

There are 36 discrepancies between the modelled and reference sequences:

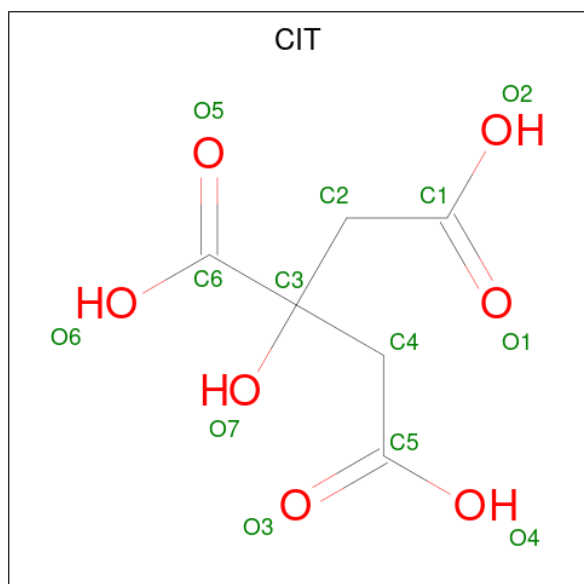
Chain	Residue	Modelled	Actual	Comment	Reference
A	112	GLY	-	expression tag	UNP P53965
A	113	SER	-	expression tag	UNP P53965
A	114	GLY	-	expression tag	UNP P53965
A	115	SER	-	expression tag	UNP P53965
B	112	GLY	-	expression tag	UNP P53965
B	113	SER	-	expression tag	UNP P53965
B	114	GLY	-	expression tag	UNP P53965
B	115	SER	-	expression tag	UNP P53965
C	112	GLY	-	expression tag	UNP P53965
C	113	SER	-	expression tag	UNP P53965
C	114	GLY	-	expression tag	UNP P53965

Continued on next page...

Continued from previous page...

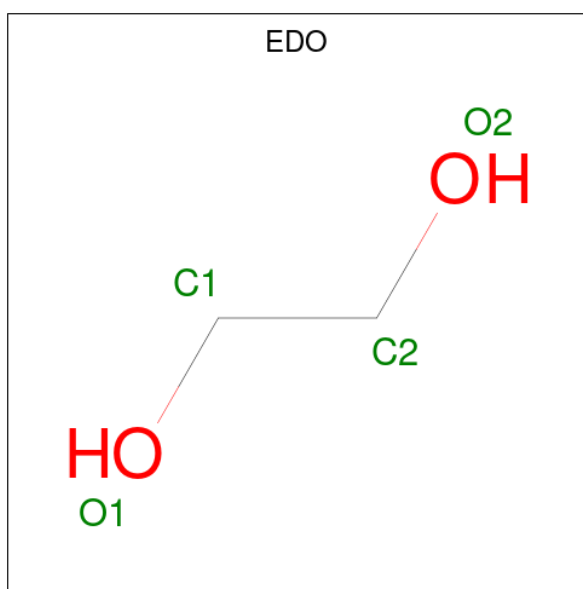
Chain	Residue	Modelled	Actual	Comment	Reference
C	115	SER	-	expression tag	UNP P53965
D	112	GLY	-	expression tag	UNP P53965
D	113	SER	-	expression tag	UNP P53965
D	114	GLY	-	expression tag	UNP P53965
D	115	SER	-	expression tag	UNP P53965
E	112	GLY	-	expression tag	UNP P53965
E	113	SER	-	expression tag	UNP P53965
E	114	GLY	-	expression tag	UNP P53965
E	115	SER	-	expression tag	UNP P53965
F	112	GLY	-	expression tag	UNP P53965
F	113	SER	-	expression tag	UNP P53965
F	114	GLY	-	expression tag	UNP P53965
F	115	SER	-	expression tag	UNP P53965
G	112	GLY	-	expression tag	UNP P53965
G	113	SER	-	expression tag	UNP P53965
G	114	GLY	-	expression tag	UNP P53965
G	115	SER	-	expression tag	UNP P53965
H	112	GLY	-	expression tag	UNP P53965
H	113	SER	-	expression tag	UNP P53965
H	114	GLY	-	expression tag	UNP P53965
H	115	SER	-	expression tag	UNP P53965
I	112	GLY	-	expression tag	UNP P53965
I	113	SER	-	expression tag	UNP P53965
I	114	GLY	-	expression tag	UNP P53965
I	115	SER	-	expression tag	UNP P53965

- 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	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		
2	E	1	Total	C	O	0	0
			13	6	7		
2	F	1	Total	C	O	0	0
			13	6	7		
2	G	1	Total	C	O	0	0
			13	6	7		
2	H	1	Total	C	O	0	0
			13	6	7		
2	I	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Cl	0	0
			1	1		
4	G	1	Total	Cl	0	0
			1	1		

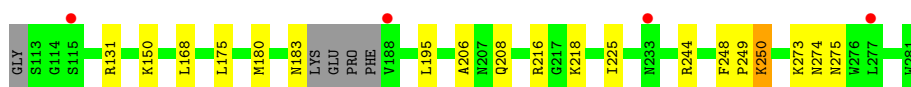
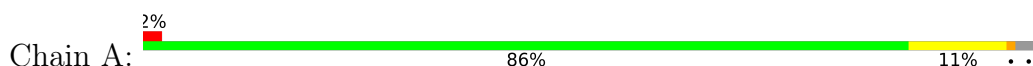
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	51	Total	O	0	0
			51	51		
5	B	47	Total	O	0	0
			47	47		
5	C	46	Total	O	0	0
			46	46		
5	D	48	Total	O	0	0
			48	48		
5	E	59	Total	O	0	0
			59	59		
5	F	36	Total	O	0	0
			36	36		
5	G	46	Total	O	0	0
			46	46		
5	H	41	Total	O	0	0
			41	41		
5	I	38	Total	O	0	0
			38	38		

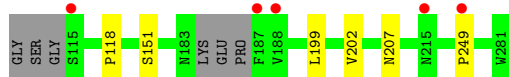
3 Residue-property plots [i](#)

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.

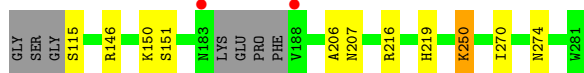
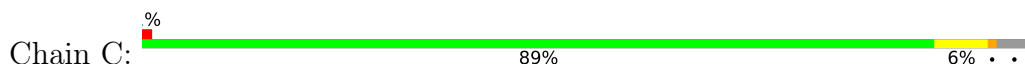
- Molecule 1: Tyrosine-protein phosphatase SIW14



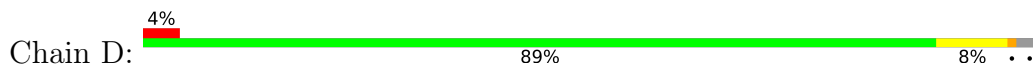
- Molecule 1: Tyrosine-protein phosphatase SIW14



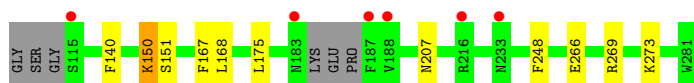
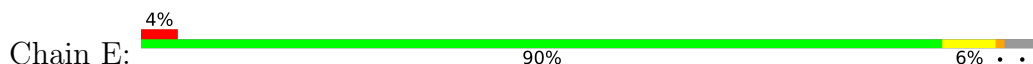
- Molecule 1: Tyrosine-protein phosphatase SIW14



- Molecule 1: Tyrosine-protein phosphatase SIW14

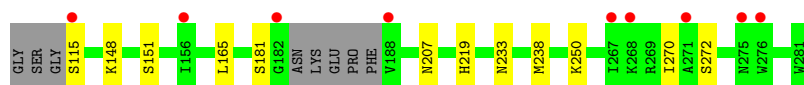


- Molecule 1: Tyrosine-protein phosphatase SIW14

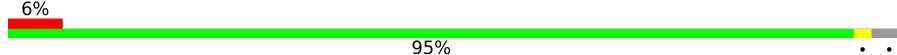


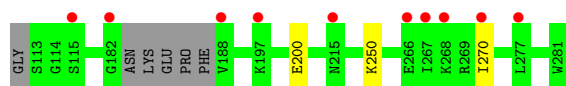
- Molecule 1: Tyrosine-protein phosphatase SIW14

Chain F:  5% 88% 7% 5%



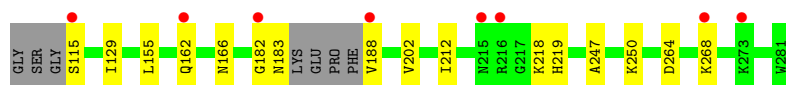
- Molecule 1: Tyrosine-protein phosphatase SIW14

Chain G:  6% 95% . .



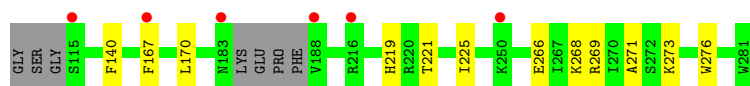
- Molecule 1: Tyrosine-protein phosphatase SIW14

Chain H:  5% 86% 9% .



- Molecule 1: Tyrosine-protein phosphatase SIW14

Chain I:  4% 89% 7% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	92.97Å 92.97Å 814.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.45 – 2.35 49.45 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.45-2.35) 92.4 (49.45-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.34Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.206 , 0.229 0.205 , 0.227	Depositor DCC
R_{free} test set	2000 reflections (2.22%)	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12692	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.85 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.0334e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, CL, EDO

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	0.26	0/1385	0.42	0/1867
1	B	0.16	0/1387	0.36	0/1870
1	C	0.39	0/1375	0.43	0/1854
1	D	0.42	0/1385	0.53	2/1867 (0.1%)
1	E	0.27	1/1387 (0.1%)	0.42	0/1870
1	F	0.30	1/1375 (0.1%)	0.51	2/1853 (0.1%)
1	G	0.16	0/1377	0.40	0/1856
1	H	0.30	0/1375	0.44	0/1854
1	I	0.29	0/1375	0.39	0/1854
All	All	0.30	2/12421 (0.0%)	0.44	4/16745 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	270	ILE	C-O	-5.18	1.18	1.24
1	E	150	LYS	C-O	-5.12	1.16	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	272	SER	CA-C-N	8.97	132.66	120.38
1	F	272	SER	C-N-CA	8.97	132.66	120.38
1	D	271	ALA	CA-C-N	5.82	128.40	120.54
1	D	271	ALA	C-N-CA	5.82	128.40	120.54

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	1355	0	1368	15	0
1	B	1356	0	1369	4	0
1	C	1345	0	1360	9	0
1	D	1355	0	1368	11	0
1	E	1356	0	1369	5	0
1	F	1345	0	1362	3	0
1	G	1347	0	1362	2	0
1	H	1345	0	1360	9	0
1	I	1345	0	1360	5	0
2	A	13	0	5	1	0
2	B	13	0	5	0	0
2	C	13	0	5	1	0
2	D	13	0	5	1	0
2	E	13	0	5	0	0
2	F	13	0	5	0	0
2	G	13	0	5	2	0
2	H	13	0	5	0	0
2	I	13	0	5	1	0
3	A	4	0	6	0	0
3	C	4	0	6	0	0
3	D	4	0	6	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
5	A	51	0	0	0	0
5	B	47	0	0	0	0
5	C	46	0	0	0	0
5	D	48	0	0	3	0
5	E	59	0	0	0	0
5	F	36	0	0	0	0
5	G	46	0	0	0	0
5	H	41	0	0	1	0
5	I	38	0	0	0	0
All	All	12692	0	12341	60	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 2.

All (60) 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:C:216:ARG:CZ	1:C:250:LYS:HE3	2.07	0.84
1:D:216:ARG:NH1	2:D:301:CIT:O2	2.24	0.70
1:C:216:ARG:NH1	1:C:250:LYS:HE3	2.07	0.69
1:A:216:ARG:NH1	2:A:301:CIT:O7	2.26	0.68
1:D:244:ARG:NE	5:D:401:HOH:O	2.33	0.62
1:D:271:ALA:HB1	1:D:276:TRP:HB2	1.84	0.60
1:D:148:LYS:NZ	5:D:402:HOH:O	2.36	0.59
1:A:150:LYS:HZ2	1:A:206:ALA:C	2.10	0.58
1:H:188:VAL:N	5:H:403:HOH:O	2.39	0.55
1:B:151:SER:OG	1:B:207:ASN:O	2.25	0.54
1:A:216:ARG:NH1	1:A:250:LYS:NZ	2.56	0.53
1:E:151:SER:OG	1:E:207:ASN:O	2.25	0.53
1:A:216:ARG:NH1	1:A:250:LYS:HZ3	2.07	0.52
1:H:155:LEU:HD21	1:H:212:ILE:HG23	1.89	0.52
1:H:202:VAL:HG11	1:H:212:ILE:HD11	1.91	0.52
1:F:151:SER:OG	1:F:207:ASN:O	2.28	0.51
1:A:150:LYS:NZ	1:A:206:ALA:C	2.70	0.50
1:G:200:GLU:OE2	1:G:270:ILE:HD13	2.13	0.49
1:A:249:PRO:HG3	1:B:249:PRO:O	2.12	0.49
1:A:216:ARG:HB3	1:A:218:LYS:HZ3	1.76	0.49
1:B:118:PRO:HG2	1:F:238[B]:MSE:HG2	1.95	0.49
1:H:182:GLY:O	1:H:183:ASN:C	2.57	0.48
1:C:270:ILE:O	1:C:274:ASN:ND2	2.46	0.48
1:C:151:SER:OG	1:C:207:ASN:O	2.30	0.48
1:A:244:ARG:NE	5:D:401:HOH:O	2.47	0.47
1:A:150:LYS:NZ	1:A:206:ALA:O	2.46	0.47
1:A:248:PHE:CZ	1:E:248:PHE:CZ	3.03	0.46
1:I:266:GLU:HG3	1:I:269:ARG:NH2	2.31	0.46
1:C:150:LYS:HE3	1:C:206:ALA:O	2.16	0.46
1:A:150:LYS:HE2	1:A:208:GLN:O	2.15	0.45
1:E:168:LEU:HD13	1:E:175:LEU:HB2	1.98	0.45
1:I:140:PHE:HB3	1:I:167:PHE:CE1	2.51	0.45
1:F:219:HIS:NE2	1:F:250:LYS:O	2.46	0.45
1:D:216:ARG:NH1	1:D:250:LYS:HE2	2.31	0.44
1:D:277:LEU:HD23	1:D:279:LEU:CD2	2.47	0.44
1:G:250:LYS:NZ	2:G:301:CIT:O4	2.42	0.44
1:A:274:ASN:O	1:A:275:ASN:HB2	2.17	0.43
1:C:146:ARG:NH2	1:D:279:LEU:O	2.51	0.43
1:H:162:GLN:OE1	1:H:166:ASN:OD1	2.37	0.43
1:B:199:LEU:HA	1:B:202:VAL:HG22	2.00	0.42
1:I:271:ALA:HB1	1:I:276:TRP:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:219:HIS:NE2	1:H:250:LYS:O	2.47	0.42
1:A:180:MSE:HE1	1:A:195:LEU:HD23	2.01	0.42
1:H:129:ILE:HD13	1:H:202:VAL:HG12	2.01	0.42
1:E:140:PHE:HB3	1:E:167:PHE:CE1	2.55	0.42
1:A:131:ARG:HD2	1:A:225:ILE:HD13	2.02	0.41
1:I:219:HIS:CE1	2:I:301:CIT:H22	2.56	0.41
1:D:218:LYS:HG2	1:D:247:ALA:HA	2.01	0.41
1:H:264:ASP:O	1:H:268:LYS:HG3	2.19	0.41
1:H:218:LYS:HG2	1:H:247:ALA:HA	2.02	0.41
1:D:271:ALA:CB	1:D:276:TRP:HB2	2.50	0.41
1:E:266:GLU:O	1:E:269:ARG:HB3	2.21	0.41
2:G:301:CIT:O1	2:G:301:CIT:C6	2.69	0.41
1:C:216:ARG:HB2	2:C:301:CIT:C5	2.51	0.40
1:C:219:HIS:HE2	1:C:250:LYS:HB3	1.86	0.40
1:D:168:LEU:HD13	1:D:175:LEU:HB2	2.04	0.40
1:D:277:LEU:HD23	1:D:279:LEU:HD22	2.03	0.40
1:A:168:LEU:HD13	1:A:175:LEU:HB2	2.04	0.40
1:C:216:ARG:CZ	1:C:250:LYS:CE	2.90	0.40
1:I:221:THR:O	1:I:225:ILE:HG12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	161/170 (95%)	155 (96%)	6 (4%)	0	100	100
1	B	160/170 (94%)	155 (97%)	5 (3%)	0	100	100
1	C	159/170 (94%)	155 (98%)	4 (2%)	0	100	100
1	D	161/170 (95%)	157 (98%)	4 (2%)	0	100	100
1	E	160/170 (94%)	155 (97%)	5 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	159/170 (94%)	154 (97%)	5 (3%)	0	100	100
1	G	160/170 (94%)	154 (96%)	6 (4%)	0	100	100
1	H	159/170 (94%)	154 (97%)	5 (3%)	0	100	100
1	I	159/170 (94%)	153 (96%)	6 (4%)	0	100	100
All	All	1438/1530 (94%)	1392 (97%)	46 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	151/152 (99%)	148 (98%)	3 (2%)	48	63
1	B	151/152 (99%)	151 (100%)	0	100	100
1	C	150/152 (99%)	148 (99%)	2 (1%)	61	76
1	D	151/152 (99%)	149 (99%)	2 (1%)	61	76
1	E	151/152 (99%)	149 (99%)	2 (1%)	61	76
1	F	150/152 (99%)	145 (97%)	5 (3%)	33	44
1	G	150/152 (99%)	150 (100%)	0	100	100
1	H	150/152 (99%)	149 (99%)	1 (1%)	76	86
1	I	150/152 (99%)	147 (98%)	3 (2%)	48	63
All	All	1354/1368 (99%)	1336 (99%)	18 (1%)	61	76

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	ASN
1	A	250	LYS
1	A	273	LYS
1	C	115	SER
1	C	250	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	188	VAL
1	D	273	LYS
1	E	150	LYS
1	E	273	LYS
1	F	115	SER
1	F	148	LYS
1	F	165	LEU
1	F	181	SER
1	F	233	ASN
1	H	115	SER
1	I	170	LEU
1	I	268	LYS
1	I	273	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	HIS
1	B	162	GLN
1	B	166	ASN
1	C	183	ASN
1	C	189	ASN
1	C	280	GLN
1	D	144	HIS
1	D	162	GLN
1	D	189	ASN
1	D	257	GLN
1	E	193	HIS
1	E	274	ASN
1	G	144	HIS
1	G	162	GLN
1	H	193	HIS
1	I	189	ASN
1	I	257	GLN

5.3.3 RNA ⓘ

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](#)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

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	F	301	-	12,12,12	1.09	0	17,17,17	1.51	2 (11%)
2	CIT	G	301	-	12,12,12	1.05	0	17,17,17	1.60	2 (11%)
2	CIT	C	301	-	12,12,12	1.04	0	17,17,17	1.85	2 (11%)
2	CIT	H	301	-	12,12,12	1.09	0	17,17,17	1.46	1 (5%)
2	CIT	A	301	-	12,12,12	1.05	0	17,17,17	1.35	1 (5%)
2	CIT	B	301	-	12,12,12	1.06	0	17,17,17	1.35	1 (5%)
2	CIT	E	301	-	12,12,12	1.09	0	17,17,17	1.43	2 (11%)
2	CIT	I	301	-	12,12,12	1.05	0	17,17,17	1.28	1 (5%)
3	EDO	C	302	-	3,3,3	0.45	0	2,2,2	0.32	0
2	CIT	D	301	-	12,12,12	1.09	0	17,17,17	1.55	2 (11%)
3	EDO	A	302	-	3,3,3	0.42	0	2,2,2	0.35	0
3	EDO	D	302	-	3,3,3	0.42	0	2,2,2	0.34	0

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	F	301	-	-	6/16/16/16	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	G	301	-	-	10/16/16/16	-
2	CIT	C	301	-	-	0/16/16/16	-
2	CIT	H	301	-	-	3/16/16/16	-
2	CIT	A	301	-	-	0/16/16/16	-
2	CIT	B	301	-	-	0/16/16/16	-
2	CIT	E	301	-	-	4/16/16/16	-
2	CIT	I	301	-	-	3/16/16/16	-
3	EDO	C	302	-	-	0/1/1/1	-
2	CIT	D	301	-	-	6/16/16/16	-
3	EDO	A	302	-	-	0/1/1/1	-
3	EDO	D	302	-	-	0/1/1/1	-

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	CIT	O6-C6-C3	5.26	123.24	113.14
2	H	301	CIT	O6-C6-C3	4.01	120.83	113.14
2	A	301	CIT	O6-C6-C3	3.94	120.70	113.14
2	G	301	CIT	O6-C6-C3	3.93	120.67	113.14
2	D	301	CIT	O6-C6-C3	3.87	120.57	113.14
2	F	301	CIT	O6-C6-C3	3.79	120.40	113.14
2	B	301	CIT	O6-C6-C3	3.76	120.36	113.14
2	I	301	CIT	O6-C6-C3	3.69	120.22	113.14
2	E	301	CIT	O6-C6-C3	3.46	119.78	113.14
2	G	301	CIT	C3-C4-C5	-2.37	107.45	113.92
2	F	301	CIT	O4-C5-C4	2.30	121.62	114.35
2	C	301	CIT	O5-C6-C3	-2.21	117.81	122.09
2	D	301	CIT	O4-C5-C4	2.13	121.08	114.35
2	E	301	CIT	O2-C1-C2	2.09	120.98	114.35

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	301	CIT	C1-C2-C3-O7
2	G	301	CIT	C1-C2-C3-C4
2	G	301	CIT	C2-C3-C4-C5
2	G	301	CIT	C6-C3-C4-C5
2	G	301	CIT	O7-C3-C6-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	G	301	CIT	O7-C3-C6-O6
2	G	301	CIT	C4-C3-C6-O5
2	G	301	CIT	C4-C3-C6-O6
2	I	301	CIT	C1-C2-C3-O7
2	I	301	CIT	C1-C2-C3-C4
2	G	301	CIT	C1-C2-C3-C6
2	G	301	CIT	O7-C3-C4-C5
2	I	301	CIT	C1-C2-C3-C6
2	H	301	CIT	C1-C2-C3-C6
2	E	301	CIT	C2-C3-C4-C5
2	H	301	CIT	C1-C2-C3-O7
2	E	301	CIT	C6-C3-C4-C5
2	F	301	CIT	C2-C3-C6-O5
2	F	301	CIT	C2-C3-C6-O6
2	F	301	CIT	C4-C3-C6-O6
2	H	301	CIT	C1-C2-C3-C4
2	F	301	CIT	C3-C4-C5-O4
2	E	301	CIT	O2-C1-C2-C3
2	D	301	CIT	C1-C2-C3-C4
2	F	301	CIT	C3-C4-C5-O3
2	F	301	CIT	C4-C3-C6-O5
2	D	301	CIT	O2-C1-C2-C3
2	D	301	CIT	C3-C4-C5-O4
2	E	301	CIT	O1-C1-C2-C3
2	D	301	CIT	C3-C4-C5-O3
2	D	301	CIT	O1-C1-C2-C3
2	D	301	CIT	C1-C2-C3-C6

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	301	CIT	2	0
2	C	301	CIT	1	0
2	A	301	CIT	1	0
2	I	301	CIT	1	0
2	D	301	CIT	1	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, 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	162/170 (95%)	0.32	4 (2%) 58 64	34, 43, 63, 74	0
1	B	161/170 (94%)	0.31	5 (3%) 51 58	34, 44, 64, 74	0
1	C	160/170 (94%)	0.25	2 (1%) 75 79	32, 43, 63, 79	0
1	D	162/170 (95%)	0.29	7 (4%) 40 45	30, 41, 61, 72	0
1	E	161/170 (94%)	0.39	6 (3%) 45 51	34, 43, 64, 75	0
1	F	159/170 (93%)	0.62	9 (5%) 29 34	36, 51, 79, 96	0
1	G	161/170 (94%)	0.44	10 (6%) 26 30	31, 43, 65, 76	0
1	H	160/170 (94%)	0.54	8 (5%) 34 40	33, 49, 68, 86	0
1	I	160/170 (94%)	0.34	6 (3%) 44 50	36, 47, 66, 79	0
All	All	1446/1530 (94%)	0.39	57 (3%) 43 49	30, 44, 67, 96	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	188	VAL	4.3
1	G	182	GLY	3.9
1	E	187	PHE	3.9
1	B	187	PHE	3.8
1	F	156	ILE	3.7
1	F	188	VAL	3.5
1	B	115	SER	3.4
1	G	115	SER	3.4
1	H	115	SER	3.4
1	C	188	VAL	3.3
1	D	115	SER	3.2
1	H	268	LYS	3.1
1	H	215	ASN	3.1
1	F	276	TRP	3.0
1	F	275	ASN	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	188	VAL	3.0
1	F	182	GLY	3.0
1	E	115	SER	3.0
1	I	115	SER	3.0
1	E	183	ASN	2.9
1	C	183	ASN	2.9
1	G	270	ILE	2.8
1	D	113	SER	2.8
1	H	162	GLN	2.7
1	H	216	ARG	2.7
1	E	233	ASN	2.7
1	F	268	LYS	2.6
1	F	115	SER	2.6
1	G	215	ASN	2.6
1	D	188	VAL	2.6
1	E	216	ARG	2.5
1	G	197	LYS	2.5
1	A	115	SER	2.5
1	A	188	VAL	2.5
1	I	167	PHE	2.4
1	I	183	ASN	2.4
1	I	216	ARG	2.4
1	D	266	GLU	2.4
1	F	271	ALA	2.4
1	E	188	VAL	2.3
1	H	273	LYS	2.3
1	H	182	GLY	2.2
1	D	269	ARG	2.2
1	A	277	LEU	2.2
1	A	233	ASN	2.2
1	B	215	ASN	2.2
1	B	249	PRO	2.2
1	G	268	LYS	2.1
1	D	277	LEU	2.1
1	G	266	GLU	2.1
1	G	267	ILE	2.1
1	B	188	VAL	2.1
1	D	215	ASN	2.1
1	F	267	ILE	2.1
1	I	188	VAL	2.1
1	I	250	LYS	2.0
1	G	277	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 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	G	301	13/13	0.62	0.16	42,59,71,73	0
2	CIT	B	301	13/13	0.68	0.15	41,60,70,75	0
2	CIT	F	301	13/13	0.76	0.13	44,58,81,85	0
2	CIT	D	301	13/13	0.77	0.12	36,54,67,67	0
2	CIT	H	301	13/13	0.78	0.12	44,55,69,71	0
2	CIT	C	301	13/13	0.82	0.12	42,58,79,80	0
2	CIT	A	301	13/13	0.84	0.10	42,55,69,69	0
2	CIT	E	301	13/13	0.85	0.12	37,56,64,68	0
2	CIT	I	301	13/13	0.88	0.10	38,49,66,74	0
3	EDO	C	302	4/4	0.95	0.08	31,32,32,35	0
3	EDO	A	302	4/4	0.97	0.08	32,34,34,40	0
3	EDO	D	302	4/4	0.97	0.08	36,37,38,38	0
4	CL	D	303	1/1	0.97	0.05	44,44,44,44	0
4	CL	G	302	1/1	0.99	0.04	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.