Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2022 – 04:20 AM EST

PDB ID	:	6BYF
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 following versions of software and data (see references ⓘ) were used in the production of this report:

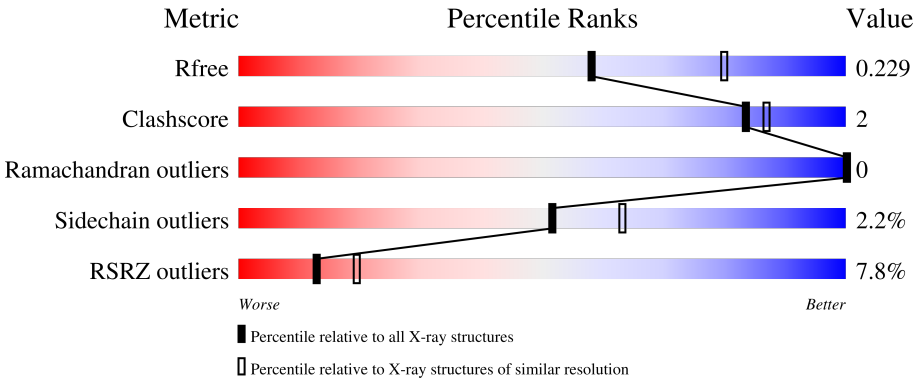
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.35 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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (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 <=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	5% 85% 11%
1	B	170	8% 91% 5%
1	C	170	5% 89% 6%
1	D	170	4% 89% 8%
1	E	170	6% 89% 7%

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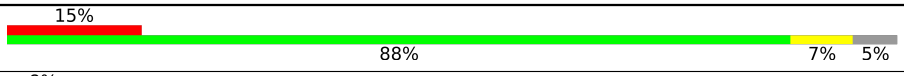
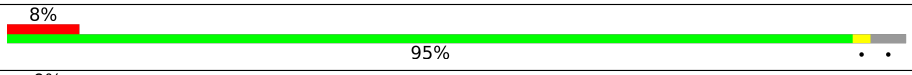
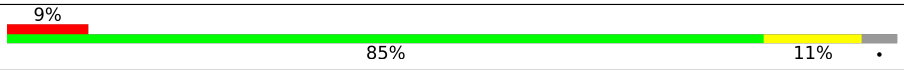
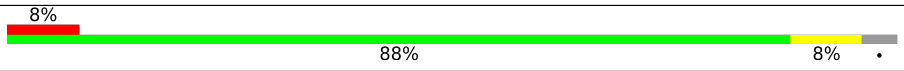
Mol	Chain	Length	Quality of chain
1	F	170	
1	G	170	
1	H	170	
1	I	170	

2 Entry composition (i)

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

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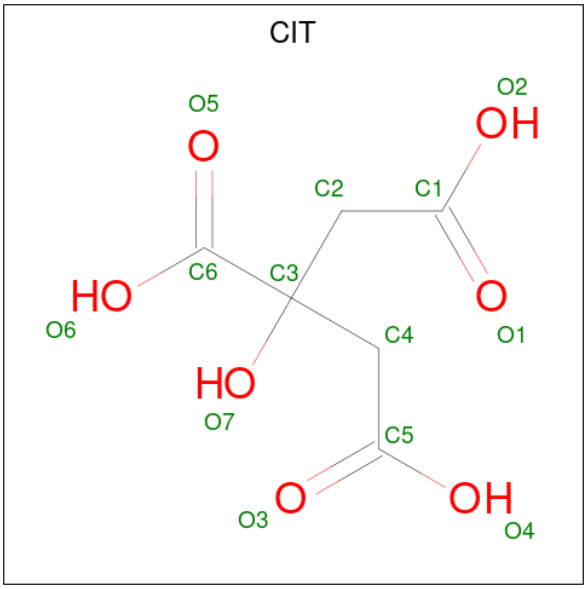
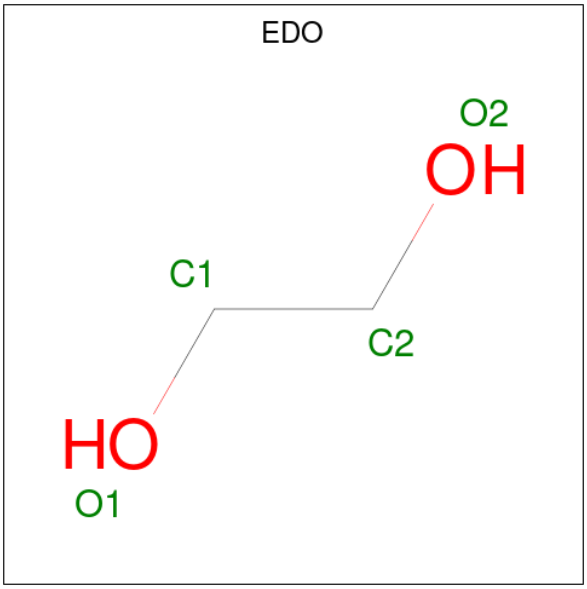
Chain	Residue	Modelled	Actual	Comment	Reference
C	115	SER	-	expression tag	UNP P53965
D	112	GLY	-	expression tag	UNP P53965
D	113	SER	-	expression tag	UNP P53965
D	114	GLY	-	expression tag	UNP P53965
D	115	SER	-	expression tag	UNP P53965
E	112	GLY	-	expression tag	UNP P53965
E	113	SER	-	expression tag	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 (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	B	1	Total C O 13 6 7	0	0
2	C	1	Total C O 13 6 7	0	0
2	D	1	Total C O 13 6 7	0	0
2	E	1	Total C O 13 6 7	0	0
2	F	1	Total C O 13 6 7	0	0
2	G	1	Total C O 13 6 7	0	0
2	H	1	Total C O 13 6 7	0	0
2	I	1	Total C O 13 6 7	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is water.

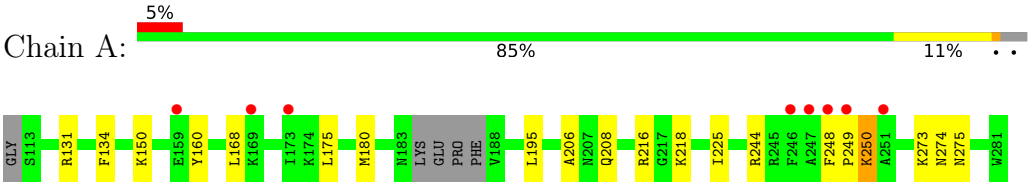
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	51	Total O 51 51	0	0
5	B	47	Total O 47 47	0	0
5	C	46	Total O 46 46	0	0
5	D	48	Total O 48 48	0	0
5	E	59	Total O 59 59	0	0
5	F	36	Total O 36 36	0	0
5	G	46	Total O 46 46	0	0
5	H	41	Total O 41 41	0	0
5	I	38	Total O 38 38	0	0

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.

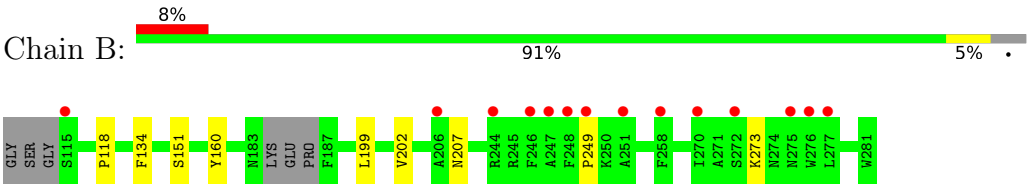
• Molecule 1: Tyrosine-protein phosphatase SIW14

Chain A:



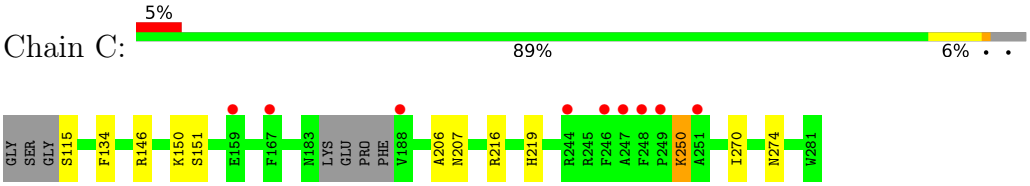
• Molecule 1: Tyrosine-protein phosphatase SIW14

Chain B:



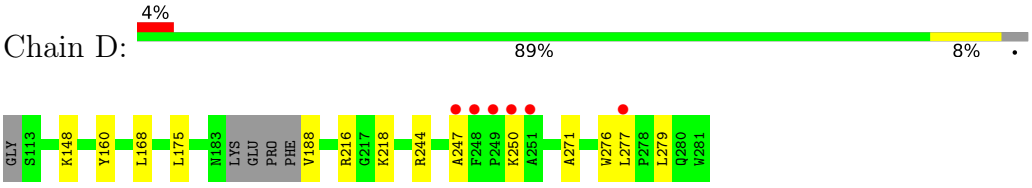
• Molecule 1: Tyrosine-protein phosphatase SIW14

Chain C:



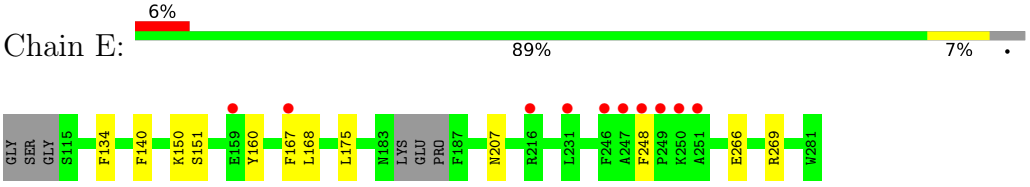
• Molecule 1: Tyrosine-protein phosphatase SIW14

Chain D:



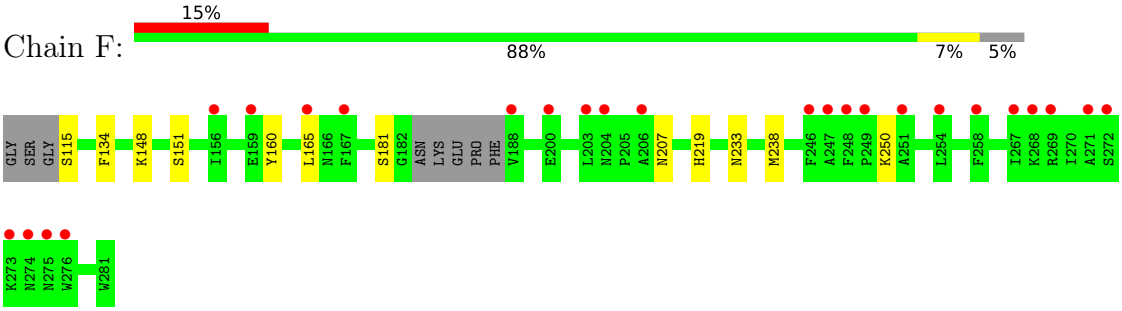
• Molecule 1: Tyrosine-protein phosphatase SIW14

Chain E:



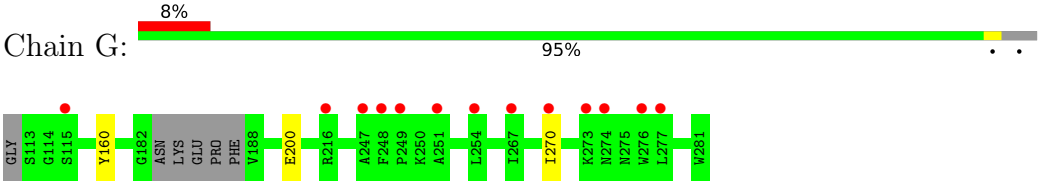
• Molecule 1: Tyrosine-protein phosphatase SIW14

Chain F:



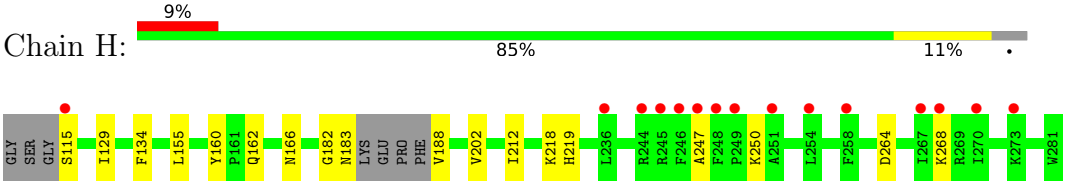
• Molecule 1: Tyrosine-protein phosphatase SIW14

Chain G:



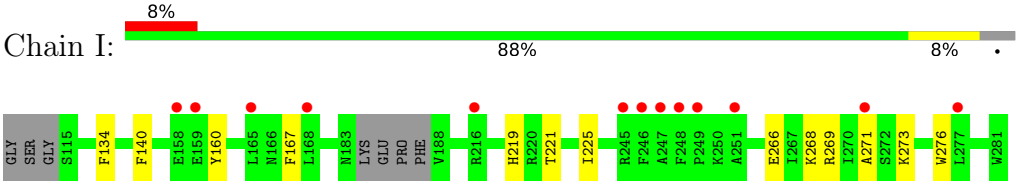
• Molecule 1: Tyrosine-protein phosphatase SIW14

Chain H:



• Molecule 1: Tyrosine-protein phosphatase SIW14

Chain I:



4 Data and refinement statistics (i)

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 – 2.34	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.45-2.35) 92.2 (49.45-2.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 2.34Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.206 , 0.229 0.206 , 0.229	Depositor DCC
R_{free} test set	1967 reflections (2.24%)	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)	0.34 , 43.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: EDO, CIT, CL

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	0.30	0/1385	0.48	0/1867
1	B	0.26	0/1387	0.45	0/1870
1	C	0.40	0/1375	0.47	0/1854
1	D	0.40	0/1385	0.49	0/1867
1	E	0.30	0/1387	0.46	0/1870
1	F	0.30	0/1375	0.48	0/1853
1	G	0.26	0/1377	0.47	0/1856
1	H	0.36	0/1375	0.48	0/1854
1	I	0.36	0/1375	0.47	0/1854
All	All	0.33	0/12421	0.47	0/16745

There are no bond length outliers.

There are no bond angle outliers.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1356	0	1369	5	0
1	F	1345	0	1362	3	0
1	G	1347	0	1362	1	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	1	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	59	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 (59) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:150:LYS:HZ2	1:A:206:ALA:C	2.10	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: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:B:118:PRO:HG2	1:F:238[B]:MSE:HG2	1.95	0.49
1:C:270:ILE:O	1:C:274:ASN:ND2	2.46	0.48
1:A:216:ARG:HB3	1:A:218:LYS:HZ3	1.77	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:NZ	1:A:206:ALA:C	2.70	0.45
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:A:274:ASN:O	1:A:275:ASN:HB2	2.17	0.43
1:H:182:GLY:O	1:H:183:ASN:C	2.57	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (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	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
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 (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	151/152 (99%)	147 (97%)	4 (3%)	46	56
1	B	151/152 (99%)	148 (98%)	3 (2%)	55	66
1	C	150/152 (99%)	147 (98%)	3 (2%)	55	66
1	D	151/152 (99%)	149 (99%)	2 (1%)	69	80
1	E	151/152 (99%)	148 (98%)	3 (2%)	55	66
1	F	150/152 (99%)	143 (95%)	7 (5%)	26	31
1	G	150/152 (99%)	149 (99%)	1 (1%)	84	91
1	H	150/152 (99%)	147 (98%)	3 (2%)	55	66
1	I	150/152 (99%)	146 (97%)	4 (3%)	44	55
All	All	1354/1368 (99%)	1324 (98%)	30 (2%)	52	63

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	PHE
1	A	160	TYR
1	A	250	LYS
1	A	273	LYS
1	B	134	PHE
1	B	160	TYR
1	B	273	LYS
1	C	115	SER
1	C	134	PHE
1	C	250	LYS
1	D	160	TYR
1	D	188	VAL
1	E	134	PHE
1	E	150	LYS
1	E	160	TYR

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Mol	Chain	Res	Type
1	F	115	SER
1	F	134	PHE
1	F	148	LYS
1	F	160	TYR
1	F	165	LEU
1	F	181	SER
1	F	233	ASN
1	G	160	TYR
1	H	115	SER
1	H	134	PHE
1	H	160	TYR
1	I	134	PHE
1	I	160	TYR
1	I	268	LYS
1	I	273	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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	C	301	-	3,12,12	1.36	0	3,17,17	1.94	2 (66%)
2	CIT	A	301	-	3,12,12	1.39	0	3,17,17	1.47	1 (33%)
2	CIT	H	301	-	3,12,12	1.52	0	3,17,17	2.18	1 (33%)
3	EDO	A	302	-	3,3,3	0.45	0	2,2,2	0.31	0
3	EDO	D	302	-	3,3,3	0.45	0	2,2,2	0.30	0
2	CIT	G	301	-	3,12,12	1.26	0	3,17,17	2.76	1 (33%)
2	CIT	B	301	-	3,12,12	1.43	0	3,17,17	1.82	1 (33%)
3	EDO	C	302	-	3,3,3	0.48	0	2,2,2	0.27	0
2	CIT	D	301	-	3,12,12	1.40	0	3,17,17	2.20	2 (66%)
2	CIT	E	301	-	3,12,12	1.20	0	3,17,17	1.96	2 (66%)
2	CIT	I	301	-	3,12,12	1.30	0	3,17,17	0.54	0
2	CIT	F	301	-	3,12,12	1.36	0	3,17,17	1.74	1 (33%)

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	C	301	-	-	0/6/16/16	-
2	CIT	A	301	-	-	0/6/16/16	-
2	CIT	H	301	-	-	3/6/16/16	-
3	EDO	A	302	-	-	0/1/1/1	-
3	EDO	D	302	-	-	0/1/1/1	-
2	CIT	G	301	-	-	6/6/16/16	-
2	CIT	B	301	-	-	1/6/16/16	-
3	EDO	C	302	-	-	0/1/1/1	-
2	CIT	D	301	-	-	1/6/16/16	-
2	CIT	E	301	-	-	1/6/16/16	-
2	CIT	I	301	-	-	4/6/16/16	-
2	CIT	F	301	-	-	0/6/16/16	-

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	301	CIT	C3-C4-C5	-4.71	107.45	114.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	301	CIT	C3-C2-C1	-3.19	109.87	114.98
2	D	301	CIT	C3-C4-C5	-2.62	110.80	114.98
2	D	301	CIT	C3-C2-C1	-2.60	110.81	114.98
2	B	301	CIT	C3-C2-C1	-2.58	110.85	114.98
2	C	301	CIT	C3-C4-C5	-2.47	111.03	114.98
2	F	301	CIT	C3-C2-C1	-2.43	111.09	114.98
2	E	301	CIT	C3-C4-C5	-2.32	111.27	114.98
2	C	301	CIT	C3-C2-C1	-2.27	111.34	114.98
2	E	301	CIT	C3-C2-C1	-2.26	111.36	114.98
2	A	301	CIT	C3-C2-C1	-2.15	111.55	114.98

There are no chirality outliers.

All (16) 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	C1-C2-C3-C6
2	G	301	CIT	C2-C3-C4-C5
2	G	301	CIT	C6-C3-C4-C5
2	H	301	CIT	C1-C2-C3-C6
2	I	301	CIT	C1-C2-C3-O7
2	I	301	CIT	C1-C2-C3-C6
2	I	301	CIT	C1-C2-C3-C4
2	G	301	CIT	O7-C3-C4-C5
2	E	301	CIT	C2-C3-C4-C5
2	H	301	CIT	C1-C2-C3-O7
2	B	301	CIT	C1-C2-C3-C6
2	I	301	CIT	C6-C3-C4-C5
2	H	301	CIT	C1-C2-C3-C4
2	D	301	CIT	C1-C2-C3-C4

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	CIT	1	0
2	A	301	CIT	1	0
2	G	301	CIT	1	0
2	D	301	CIT	1	0
2	I	301	CIT	1	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, 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	162/170 (95%)	0.41	8 (4%) 29 42	34, 43, 63, 74	0
1	B	161/170 (94%)	0.50	14 (8%) 10 15	34, 44, 64, 74	0
1	C	160/170 (94%)	0.42	9 (5%) 24 35	32, 43, 63, 79	0
1	D	162/170 (95%)	0.34	6 (3%) 41 54	30, 41, 61, 72	0
1	E	161/170 (94%)	0.46	10 (6%) 20 29	34, 43, 64, 75	0
1	F	159/170 (93%)	0.77	25 (15%) 2 3	36, 51, 79, 96	0
1	G	161/170 (94%)	0.57	13 (8%) 12 17	31, 43, 65, 76	0
1	H	160/170 (94%)	0.58	15 (9%) 8 13	33, 49, 68, 86	0
1	I	160/170 (94%)	0.42	13 (8%) 12 17	36, 47, 66, 79	0
All	All	1446/1530 (94%)	0.50	113 (7%) 13 19	30, 44, 67, 96	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	249	PRO	6.1
1	A	248	PHE	5.6
1	I	248	PHE	5.6
1	A	249	PRO	5.5
1	D	249	PRO	5.4
1	G	249	PRO	5.3
1	F	275	ASN	5.2
1	C	249	PRO	5.2
1	E	249	PRO	5.0
1	C	248	PHE	4.9
1	I	249	PRO	4.9
1	H	248	PHE	4.7
1	G	270	ILE	4.6
1	C	188	VAL	4.6
1	E	248	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	277	LEU	4.5
1	D	248	PHE	4.4
1	F	271	ALA	4.2
1	A	247	ALA	4.2
1	F	249	PRO	4.1
1	G	277	LEU	4.1
1	B	248	PHE	4.0
1	F	206	ALA	3.9
1	F	248	PHE	3.9
1	I	251	ALA	3.7
1	B	270	ILE	3.7
1	F	159	GLU	3.7
1	F	247	ALA	3.7
1	G	251	ALA	3.6
1	H	251	ALA	3.6
1	F	268	LYS	3.6
1	A	251	ALA	3.6
1	G	248	PHE	3.5
1	F	276	TRP	3.3
1	B	247	ALA	3.2
1	D	247	ALA	3.1
1	I	168	LEU	3.1
1	A	246	PHE	3.1
1	B	251	ALA	3.1
1	C	251	ALA	3.0
1	E	251	ALA	3.0
1	E	159	GLU	3.0
1	I	246	PHE	2.9
1	H	268	LYS	2.9
1	H	249	PRO	2.9
1	I	277	LEU	2.9
1	D	251	ALA	2.7
1	G	247	ALA	2.7
1	G	273	LYS	2.7
1	B	115	SER	2.7
1	A	159	GLU	2.7
1	I	247	ALA	2.7
1	H	258	PHE	2.6
1	C	247	ALA	2.6
1	F	272	SER	2.6
1	C	244	ARG	2.6
1	E	246	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	246	PHE	2.5
1	F	246	PHE	2.5
1	F	203	LEU	2.5
1	B	276	TRP	2.5
1	G	276	TRP	2.5
1	E	247	ALA	2.5
1	F	267	ILE	2.5
1	F	269	ARG	2.5
1	F	204	ASN	2.5
1	I	159	GLU	2.5
1	F	165	LEU	2.5
1	C	167	PHE	2.4
1	C	246	PHE	2.4
1	H	236	LEU	2.4
1	B	206	ALA	2.4
1	G	216	ARG	2.4
1	H	115	SER	2.4
1	H	273	LYS	2.4
1	G	267	ILE	2.3
1	I	165	LEU	2.3
1	G	115	SER	2.3
1	D	250	LYS	2.3
1	E	231	LEU	2.3
1	H	244	ARG	2.3
1	E	250	LYS	2.3
1	A	169	LYS	2.2
1	F	251	ALA	2.2
1	E	167	PHE	2.2
1	F	258	PHE	2.2
1	I	216	ARG	2.2
1	F	156	ILE	2.2
1	H	267	ILE	2.2
1	H	254	LEU	2.2
1	F	274	ASN	2.2
1	H	270	ILE	2.2
1	C	159	GLU	2.2
1	F	273	LYS	2.2
1	H	247	ALA	2.2
1	B	275	ASN	2.1
1	G	254	LEU	2.1
1	F	167	PHE	2.1
1	F	254	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	216	ARG	2.1
1	D	277	LEU	2.1
1	F	200	GLU	2.1
1	I	245	ARG	2.1
1	G	274	ASN	2.1
1	I	158	GLU	2.1
1	B	244	ARG	2.1
1	F	188	VAL	2.1
1	A	173	ILE	2.0
1	H	245	ARG	2.0
1	B	272	SER	2.0
1	B	258	PHE	2.0
1	H	246	PHE	2.0
1	I	271	ALA	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 monosaccharides 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, 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	B-factors(Å^2)	Q<0.9
2	CIT	G	301	13/13	0.75	0.20	42,59,71,73	0
2	CIT	B	301	13/13	0.78	0.23	41,60,70,75	0
2	CIT	C	301	13/13	0.84	0.19	42,58,79,80	0
2	CIT	H	301	13/13	0.85	0.16	44,55,69,71	0
2	CIT	F	301	13/13	0.87	0.17	44,58,81,85	0
2	CIT	D	301	13/13	0.88	0.16	36,54,67,67	0
2	CIT	A	301	13/13	0.89	0.13	42,55,69,69	0
2	CIT	I	301	13/13	0.89	0.15	38,49,66,74	0
2	CIT	E	301	13/13	0.90	0.15	37,56,64,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	A	302	4/4	0.91	0.28	32,34,34,40	0
3	EDO	D	302	4/4	0.93	0.20	36,37,38,38	0
3	EDO	C	302	4/4	0.96	0.18	31,32,32,35	0
4	CL	D	303	1/1	0.96	0.05	44,44,44,44	0
4	CL	G	302	1/1	0.96	0.09	41,41,41,41	0

6.5 Other polymers

There are no such residues in this entry.