WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jun 7, 2020 – 02:32 am BST

PDB ID	:	6HSU
Title	:	The crystal structure of type II Dehydroquinase from Psychromonas ingrahamii 37, crystal form 2
Authors	:	Lapthorn, A.J.; Roszak, A.W.
Deposited on	:	2018-10-01
Resolution	:	1.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

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

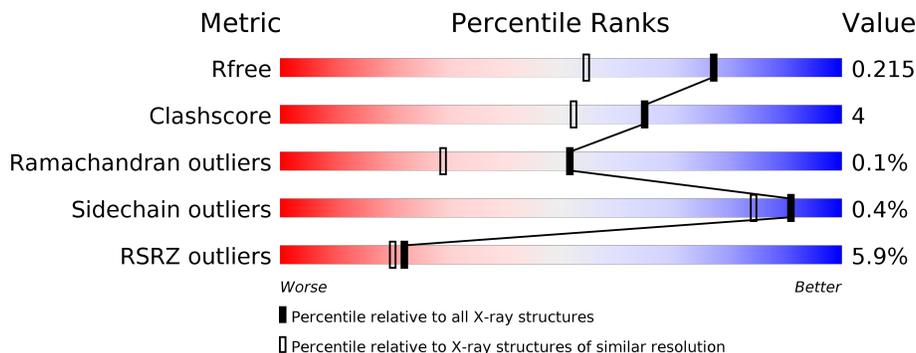|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.60 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.
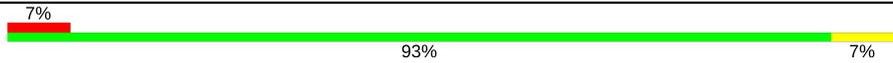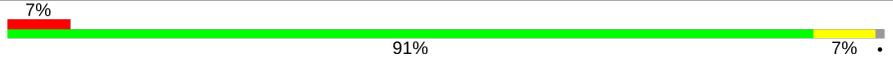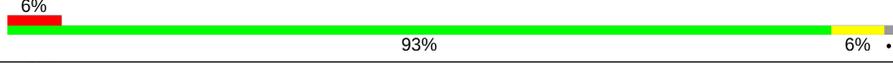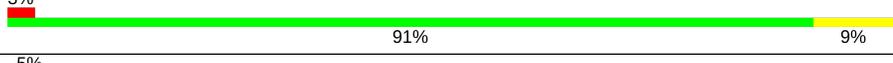
Metric	Percentile Ranks	Value
Rfree		0.215
Clashscore		4
Ramachandran outliers		0.1%
Sidechain outliers		0.4%
RSRZ outliers		5.9%

Worse ← → *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 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	152	7% / 88% / 10% ·
1	B	152	6% / 89% / 10% ·
1	C	152	3% / 91% / 7% ·
1	D	152	5% / 91% / 9%
1	E	152	7% / 89% / 9% ·
1	F	152	7% / 91% / 8% ·

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	152	7% 93% 7%
1	H	152	7% 91% 7%
1	I	152	6% 93% 6%
1	J	152	7% 87% 13%
1	K	152	3% 91% 9%
1	L	152	5% 91% 7%
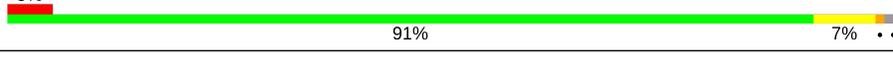
2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15740 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 3-dehydroquinate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	148	Total	C	N	O	S	0	1	0
			1150	734	203	212	1			
1	B	150	Total	C	N	O	S	0	4	0
			1186	758	207	219	2			
1	C	150	Total	C	N	O	S	0	8	0
			1201	766	210	224	1			
1	D	152	Total	C	N	O	S	0	7	0
			1215	776	212	225	2			
1	E	148	Total	C	N	O	S	0	2	0
			1147	730	204	212	1			
1	F	151	Total	C	N	O	S	0	4	0
			1192	762	210	218	2			
1	G	152	Total	C	N	O	S	0	4	0
			1195	762	209	222	2			
1	H	150	Total	C	N	O	S	0	1	0
			1164	741	205	217	1			
1	I	150	Total	C	N	O	S	0	2	0
			1175	751	207	215	2			
1	J	151	Total	C	N	O	S	0	5	0
			1191	761	209	219	2			
1	K	151	Total	C	N	O	S	0	7	0
			1205	771	210	222	2			
1	L	149	Total	C	N	O	S	0	3	0
			1168	743	206	218	1			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A1SZA3
A	-1	SER	-	expression tag	UNP A1SZA3
A	0	HIS	-	expression tag	UNP A1SZA3
B	-2	GLY	-	expression tag	UNP A1SZA3
B	-1	SER	-	expression tag	UNP A1SZA3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	HIS	-	expression tag	UNP A1SZA3
C	-2	GLY	-	expression tag	UNP A1SZA3
C	-1	SER	-	expression tag	UNP A1SZA3
C	0	HIS	-	expression tag	UNP A1SZA3
D	-2	GLY	-	expression tag	UNP A1SZA3
D	-1	SER	-	expression tag	UNP A1SZA3
D	0	HIS	-	expression tag	UNP A1SZA3
E	-2	GLY	-	expression tag	UNP A1SZA3
E	-1	SER	-	expression tag	UNP A1SZA3
E	0	HIS	-	expression tag	UNP A1SZA3
F	-2	GLY	-	expression tag	UNP A1SZA3
F	-1	SER	-	expression tag	UNP A1SZA3
F	0	HIS	-	expression tag	UNP A1SZA3
G	-2	GLY	-	expression tag	UNP A1SZA3
G	-1	SER	-	expression tag	UNP A1SZA3
G	0	HIS	-	expression tag	UNP A1SZA3
H	-2	GLY	-	expression tag	UNP A1SZA3
H	-1	SER	-	expression tag	UNP A1SZA3
H	0	HIS	-	expression tag	UNP A1SZA3
I	-2	GLY	-	expression tag	UNP A1SZA3
I	-1	SER	-	expression tag	UNP A1SZA3
I	0	HIS	-	expression tag	UNP A1SZA3
J	-2	GLY	-	expression tag	UNP A1SZA3
J	-1	SER	-	expression tag	UNP A1SZA3
J	0	HIS	-	expression tag	UNP A1SZA3
K	-2	GLY	-	expression tag	UNP A1SZA3
K	-1	SER	-	expression tag	UNP A1SZA3
K	0	HIS	-	expression tag	UNP A1SZA3
L	-2	GLY	-	expression tag	UNP A1SZA3
L	-1	SER	-	expression tag	UNP A1SZA3
L	0	HIS	-	expression tag	UNP A1SZA3

- Molecule 2 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).
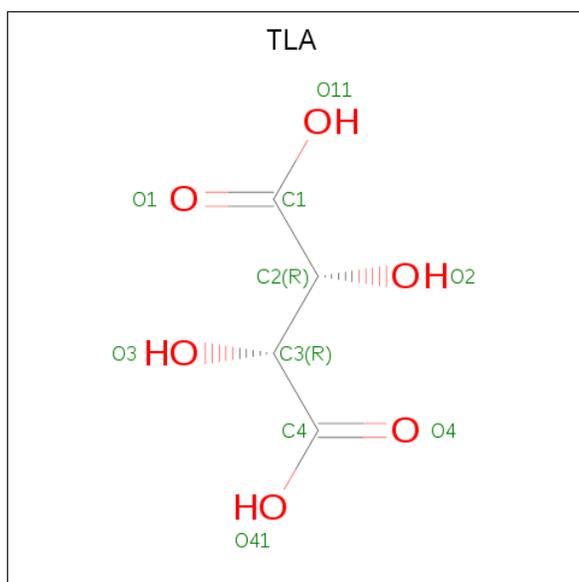
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 10	C 4	O 6	0	0
2	B	1	Total 10	C 4	O 6	0	0
2	C	1	Total 10	C 4	O 6	0	0
2	D	1	Total 10	C 4	O 6	0	0
2	E	1	Total 10	C 4	O 6	0	0
2	F	1	Total 10	C 4	O 6	0	0
2	G	1	Total 10	C 4	O 6	0	0
2	H	1	Total 10	C 4	O 6	0	0
2	I	1	Total 10	C 4	O 6	0	0
2	J	1	Total 10	C 4	O 6	0	0
2	K	1	Total 10	C 4	O 6	0	0
2	L	1	Total 10	C 4	O 6	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
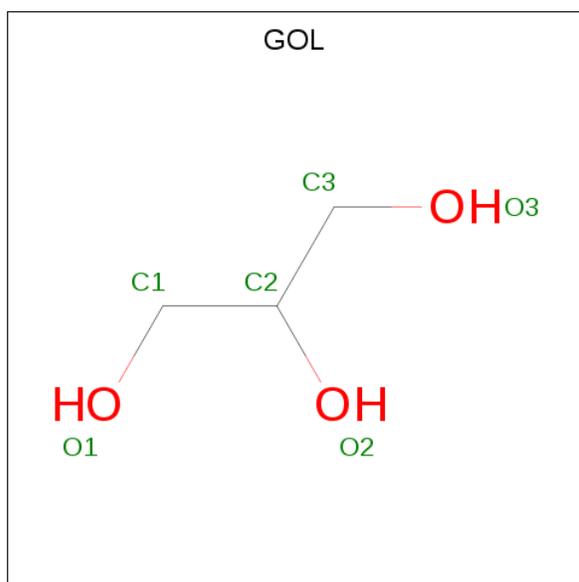
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 6	C 3	O 3	0	0

- Molecule 4 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: $C_7H_{15}NO_4S$).
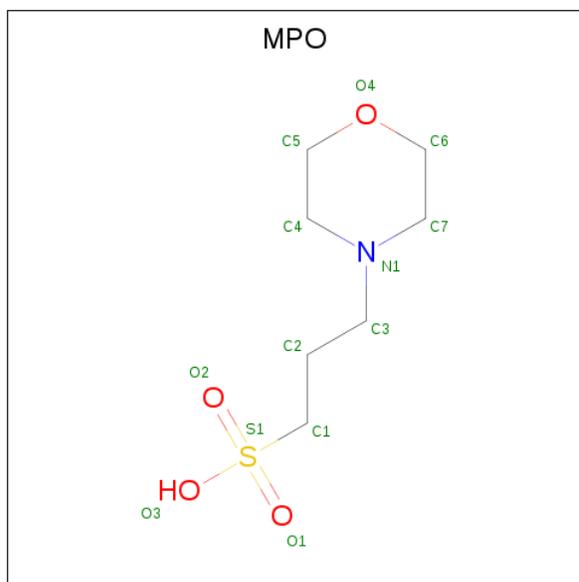
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	K	1	Total 13	C 7	N 1	O 4	S 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	88	Total 88	O 88	0	0
5	B	125	Total 125	O 125	0	0
5	C	134	Total 134	O 134	0	0
5	D	123	Total 123	O 123	0	0
5	E	95	Total 95	O 95	0	0
5	F	139	Total 139	O 139	0	0
5	G	117	Total 117	O 117	0	0
5	H	96	Total 96	O 96	0	0
5	I	117	Total 117	O 117	0	0
5	J	131	Total 131	O 131	0	0
5	K	133	Total 133	O 133	0	0
5	L	114	Total 114	O 114	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 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: 3-dehydroquinate dehydratase
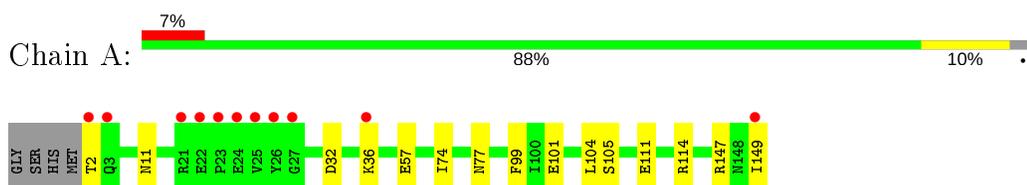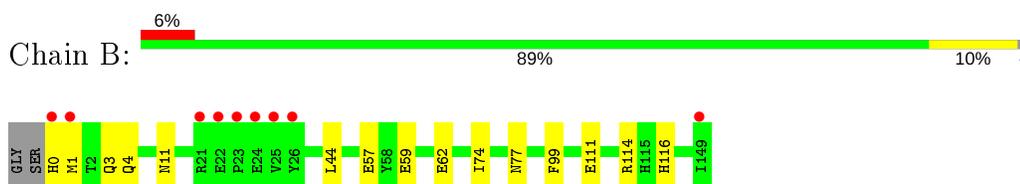
- Molecule 1: 3-dehydroquinate dehydratase

- Molecule 1: 3-dehydroquinate dehydratase

- Molecule 1: 3-dehydroquinate dehydratase

- Molecule 1: 3-dehydroquinate dehydratase

- Molecule 1: 3-dehydroquinate dehydratase

Chain F:

7%

91%

8%

GLY | S-1 | H0 | M1 | N11 | R21 | E22 | P23 | E24 | V25 | Y26 | G27 | E57 | E62 | I74 | N77 | P78 | A79 | G94 | F99 | I100 | E101 | H116 | K133 | Q140 | N148 | I149

- Molecule 1: 3-dehydroquinate dehydratase

Chain G:

7%

93%

7%

G-2 | S-1 | H0 | M1 | T2 | Q3 | N11 | R21 | E22 | P23 | E24 | V25 | Y26 | G27 | E57 | I74 | N77 | F99 | I100 | E101 | E111 | H116 | I149

- Molecule 1: 3-dehydroquinate dehydratase

Chain H:

7%

91%

7%

GLY | SER | H0 | N11 | Q20 | R21 | E22 | E24 | V25 | Y26 | G27 | S28 | E41 | E57 | I74 | N77 | G94 | V95 | F99 | S120 | N148 | I149

- Molecule 1: 3-dehydroquinate dehydratase

Chain I:

6%

93%

6%

GLY | SER | H0 | M1 | N11 | R21 | E22 | P23 | E24 | V25 | Y26 | G27 | S28 | E57 | Y58 | E59 | I74 | N77 | P78 | A79 | F99 | K133 | G144 | I149

- Molecule 1: 3-dehydroquinate dehydratase

Chain J:

7%

87%

13%

GLY | S-1 | H0 | M1 | T2 | Q3 | Q4 | N11 | R21 | E22 | P23 | E24 | V25 | Y26 | G27 | S28 | K29 | D32 | K36 | E57 | E62 | I74 | N77 | P78 | A79 | F99 | I100 | E101 | E111 | R114 | H115 | H116 | K133 | Q140 | I149

- Molecule 1: 3-dehydroquinate dehydratase

Chain K:

3%

91%

9%

GLY | S-1 | Q3 | N11 | E22 | P23 | E24 | V25 | Y26 | E41 | E57 | E62 | D72 | F73 | I74 | N77 | P78 | A79 | G94 | F99 | I100 | E101 | I149

- Molecule 1: 3-dehydroquinate dehydratase

Chain L:

5%

91%

7%

GLY | SER | HIS | M1 | T2 | Q3 | N11 | E22 | V25 | Y26 | G27 | S28 | E57 | E62 | D66 | I74 | N77 | F99 | E111 | K133 | N148 | I149
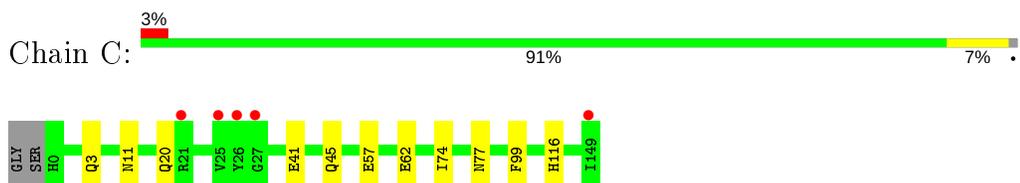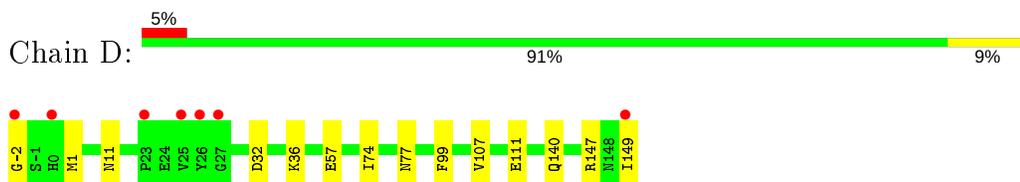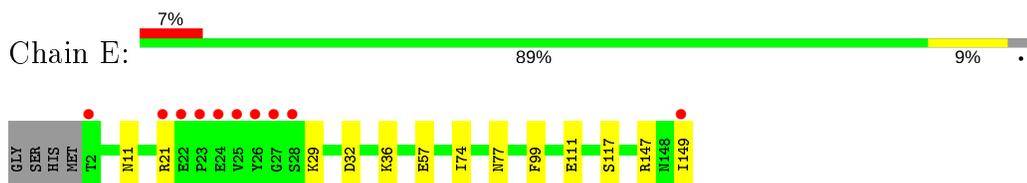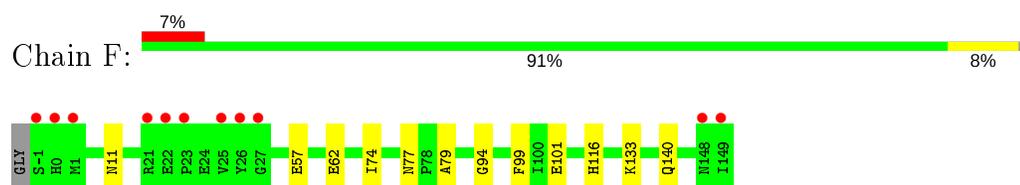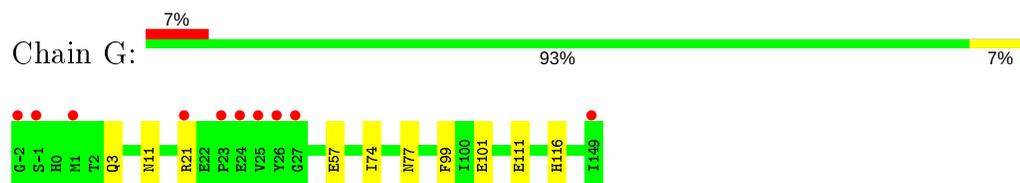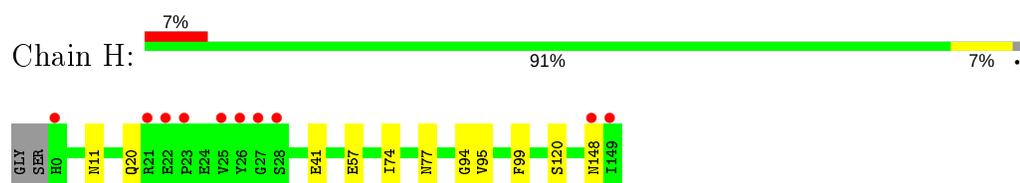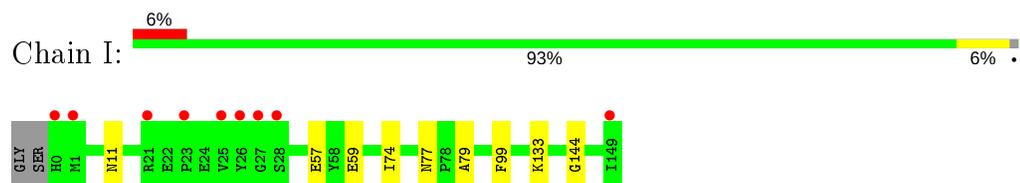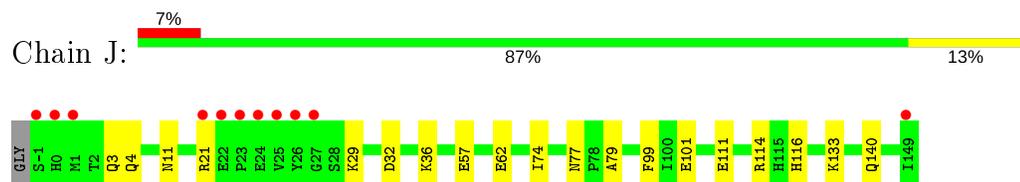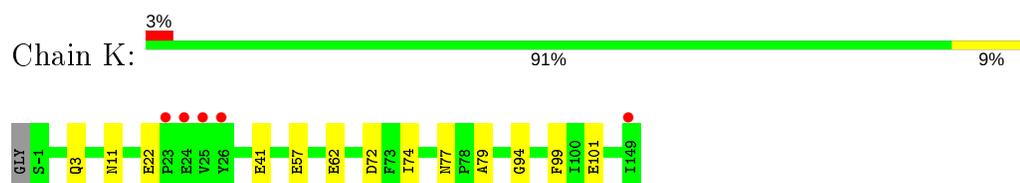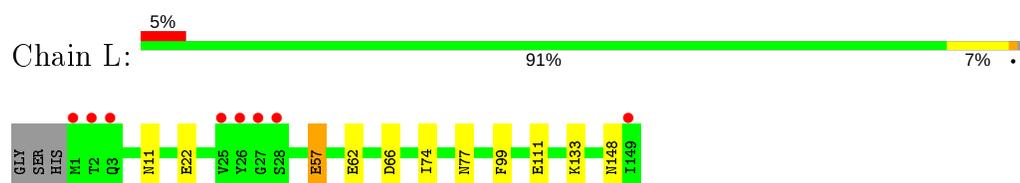
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	137.57Å　　137.95Å　　139.42Å 90.00°　　　90.00°　　　90.00°	Depositor
Resolution (Å)	79.98　–　1.60 79.85　–　1.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (79.98-1.60) 99.6 (79.85-1.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.32 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.191　,　0.208 0.199　,　0.215	Depositor DCC
R_{free} test set	17403 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	25.1	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 49.8	EDS
L-test for twinning [2]	$<|L|> = 0.45$, $<L^2> = 0.28$	Xtriage
Estimated twinning fraction	0.035 for -h,l,k 0.036 for -l,-k,-h 0.036 for k,h,-l 0.074 for k,l,h 0.074 for l,h,k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15740	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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, 0.333 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: GOL, TLA, MPO

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	0.85	2/1173 (0.2%)	0.82	1/1588 (0.1%)
1	B	0.91	2/1218 (0.2%)	0.88	1/1648 (0.1%)
1	C	0.95	3/1246 (0.2%)	0.86	0/1687
1	D	0.87	2/1257 (0.2%)	0.85	0/1699
1	E	0.85	2/1172 (0.2%)	0.82	0/1586
1	F	0.96	3/1225 (0.2%)	0.84	0/1658
1	G	0.87	2/1228 (0.2%)	0.83	0/1662
1	H	0.84	2/1187 (0.2%)	0.80	0/1607
1	I	0.88	1/1202 (0.1%)	0.81	0/1627
1	J	0.94	3/1226 (0.2%)	0.84	1/1658 (0.1%)
1	K	0.95	5/1247 (0.4%)	0.85	0/1686
1	L	0.83	2/1196 (0.2%)	0.82	0/1617
All	All	0.89	29/14577 (0.2%)	0.84	3/19723 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	57	GLU	CD-OE2	11.43	1.38	1.25
1	F	57	GLU	CD-OE2	9.97	1.36	1.25
1	A	57	GLU	CD-OE2	9.78	1.36	1.25
1	C	57	GLU	CD-OE2	9.78	1.36	1.25
1	I	57	GLU	CD-OE2	9.76	1.36	1.25

wwPDB X-ray Structure Validation Summary Report

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	114	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	A	114	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	J	114	ARG	NE-CZ-NH2	-5.66	117.47	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	0	HIS	Mainchain,Peptide

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	1150	0	1163	10	1
1	B	1186	0	1213	11	0
1	C	1201	0	1222	6	0
1	D	1215	0	1248	15	0
1	E	1147	0	1157	11	0
1	F	1192	0	1216	9	0
1	G	1195	0	1214	7	0
1	H	1164	0	1172	7	0
1	I	1175	0	1198	7	0
1	J	1191	0	1218	22	0
1	K	1205	0	1240	7	0
1	L	1168	0	1188	7	0
2	A	10	0	4	1	0
2	B	10	0	3	0	0
2	C	10	0	4	0	0
2	D	10	0	4	0	0
2	E	10	0	4	0	0
2	F	10	0	4	2	0
2	G	10	0	4	0	0
2	H	10	0	4	0	0
2	I	10	0	4	1	0
2	J	10	0	3	1	0

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	10	0	4	1	0
2	L	10	0	4	0	0
3	B	6	0	8	2	0
4	K	13	0	14	2	0
5	A	88	0	0	3	0
5	B	125	0	0	4	0
5	C	134	0	0	4	0
5	D	123	0	0	3	0
5	E	95	0	0	5	0
5	F	139	0	0	5	0
5	G	117	0	0	3	0
5	H	96	0	0	3	1
5	I	117	0	0	2	0
5	J	131	0	0	9	0
5	K	133	0	0	0	0
5	L	114	0	0	3	0
All	All	15740	0	14517	117	1

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 4.

The worst 5 of 117 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:D:140[A]:GLN:NE2	5:D:303:HOH:O	1.61	1.31
1:J:140[A]:GLN:NE2	5:J:303:HOH:O	1.56	1.28
1:B:116:HIS:ND1	5:B:303:HOH:O	1.86	1.07
1:J:111:GLU:OE2	5:J:304:HOH:O	1.83	0.94
1:F:116:HIS:CD2	5:F:319:HOH:O	2.19	0.93

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:THR:CB	5:H:389:HOH:O[4_456]	1.90	0.30

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	147/152 (97%)	144 (98%)	3 (2%)	0	100	100
1	B	152/152 (100%)	148 (97%)	3 (2%)	1 (1%)	22	7
1	C	156/152 (103%)	153 (98%)	3 (2%)	0	100	100
1	D	157/152 (103%)	154 (98%)	3 (2%)	0	100	100
1	E	148/152 (97%)	145 (98%)	3 (2%)	0	100	100
1	F	153/152 (101%)	151 (99%)	2 (1%)	0	100	100
1	G	154/152 (101%)	151 (98%)	3 (2%)	0	100	100
1	H	149/152 (98%)	146 (98%)	3 (2%)	0	100	100
1	I	150/152 (99%)	147 (98%)	3 (2%)	0	100	100
1	J	154/152 (101%)	151 (98%)	3 (2%)	0	100	100
1	K	156/152 (103%)	153 (98%)	3 (2%)	0	100	100
1	L	150/152 (99%)	147 (98%)	3 (2%)	0	100	100
All	All	1826/1824 (100%)	1790 (98%)	35 (2%)	1 (0%)	51	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1	MET

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	123/128 (96%)	123 (100%)	0	100	100
1	B	129/128 (101%)	129 (100%)	0	100	100
1	C	132/128 (103%)	131 (99%)	1 (1%)	81	70
1	D	134/128 (105%)	134 (100%)	0	100	100
1	E	122/128 (95%)	121 (99%)	1 (1%)	81	70
1	F	129/128 (101%)	129 (100%)	0	100	100
1	G	130/128 (102%)	129 (99%)	1 (1%)	81	70
1	H	124/128 (97%)	123 (99%)	1 (1%)	81	70
1	I	127/128 (99%)	127 (100%)	0	100	100
1	J	129/128 (101%)	129 (100%)	0	100	100
1	K	133/128 (104%)	133 (100%)	0	100	100
1	L	126/128 (98%)	124 (98%)	2 (2%)	62	41
All	All	1538/1536 (100%)	1532 (100%)	6 (0%)	91	84

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	3	GLN
1	L	148	ASN
1	H	148	ASN
1	E	29	LYS
1	L	22	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	115	HIS
1	H	115	HIS
1	L	115	HIS
1	H	11	ASN
1	H	116	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

14 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	TLA	C	201	-	3,9,9	1.18	0	6,12,12	3.55	5 (83%)
2	TLA	E	201	-	3,9,9	1.77	1 (33%)	6,12,12	3.06	4 (66%)
3	GOL	B	202	-	5,5,5	0.12	0	5,5,5	0.47	0
2	TLA	A	201	-	3,9,9	1.32	0	6,12,12	2.46	3 (50%)
2	TLA	K	201	-	3,9,9	1.08	0	6,12,12	3.17	3 (50%)
2	TLA	D	201	-	3,9,9	1.38	1 (33%)	6,12,12	3.29	3 (50%)
2	TLA	I	201	-	3,9,9	1.44	0	6,12,12	3.50	4 (66%)
2	TLA	F	201	-	3,9,9	1.70	1 (33%)	6,12,12	2.91	2 (33%)
4	MPO	K	202	-	13,13,13	1.11	1 (7%)	17,17,17	0.94	2 (11%)
2	TLA	B	201	-	3,9,9	1.66	1 (33%)	6,12,12	4.48	5 (83%)
2	TLA	L	201	-	3,9,9	1.50	0	6,12,12	3.31	4 (66%)
2	TLA	H	201	-	3,9,9	0.95	0	6,12,12	3.28	3 (50%)
2	TLA	J	201	-	3,9,9	1.45	1 (33%)	6,12,12	4.61	6 (100%)
2	TLA	G	201	-	3,9,9	1.14	0	6,12,12	1.78	1 (16%)

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	TLA	C	201	-	-	2/4/12/12	-
2	TLA	E	201	-	-	1/4/12/12	-
3	GOL	B	202	-	-	2/4/4/4	-
2	TLA	A	201	-	-	0/4/12/12	-
2	TLA	K	201	-	-	3/4/12/12	-
2	TLA	D	201	-	-	2/4/12/12	-
2	TLA	I	201	-	-	2/4/12/12	-
2	TLA	F	201	-	-	3/4/12/12	-
4	MPO	K	202	-	-	0/7/15/15	0/1/1/1
2	TLA	B	201	-	-	2/4/12/12	-
2	TLA	L	201	-	-	2/4/12/12	-
2	TLA	H	201	-	-	2/4/12/12	-
2	TLA	J	201	-	-	2/4/12/12	-
2	TLA	G	201	-	-	2/4/12/12	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	202	MPO	O1-S1	3.80	1.56	1.45
2	B	201	TLA	C3-C2	2.80	1.63	1.53
2	J	201	TLA	C3-C2	2.23	1.61	1.53
2	E	201	TLA	C3-C2	2.20	1.60	1.53
2	F	201	TLA	O3-C3	-2.16	1.38	1.42

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	201	TLA	O2-C2-C1	-7.16	93.86	111.10
2	I	201	TLA	C4-C3-C2	6.49	127.08	113.11
2	L	201	TLA	C4-C3-C2	6.42	126.92	113.11
2	B	201	TLA	C4-C3-C2	6.23	126.51	113.11
2	F	201	TLA	C4-C3-C2	6.19	126.43	113.11

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	201	TLA	C1-C2-C3-C4
2	K	201	TLA	C1-C2-C3-C4
2	K	201	TLA	O2-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	201	TLA	C1-C2-C3-C4
2	I	201	TLA	C1-C2-C3-C4

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	202	GOL	2	0
2	A	201	TLA	1	0
2	K	201	TLA	1	0
2	I	201	TLA	1	0
2	F	201	TLA	2	0
4	K	202	MPO	2	0
2	J	201	TLA	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	148/152 (97%)	0.25	11 (7%)	14	13	24, 34, 81, 116	1 (0%)
1	B	150/152 (98%)	0.06	9 (6%)	21	19	19, 26, 72, 96	0
1	C	150/152 (98%)	0.03	5 (3%)	46	43	19, 25, 58, 83	0
1	D	152/152 (100%)	-0.03	7 (4%)	32	29	21, 27, 59, 88	0
1	E	148/152 (97%)	0.27	10 (6%)	17	16	22, 30, 71, 129	1 (0%)
1	F	151/152 (99%)	0.12	11 (7%)	15	13	19, 25, 71, 100	1 (0%)
1	G	152/152 (100%)	0.10	10 (6%)	18	17	21, 28, 72, 120	0
1	H	150/152 (98%)	0.20	10 (6%)	17	16	24, 32, 72, 97	1 (0%)
1	I	150/152 (98%)	0.02	9 (6%)	21	19	20, 29, 71, 91	1 (0%)
1	J	151/152 (99%)	0.10	11 (7%)	15	13	19, 26, 74, 114	1 (0%)
1	K	151/152 (99%)	-0.02	5 (3%)	46	43	19, 25, 62, 87	1 (0%)
1	L	149/152 (98%)	0.03	8 (5%)	25	23	20, 26, 64, 91	1 (0%)
All	All	1802/1824 (98%)	0.10	106 (5%)	22	20	19, 28, 72, 129	8 (0%)

The worst 5 of 106 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	25	VAL	18.5
1	H	25	VAL	12.0
1	C	149	ILE	10.9
1	G	27	GLY	9.8
1	F	149	ILE	9.0

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. 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(Å^2)	Q<0.9
2	TLA	G	201	10/10	0.79	0.31	31,49,55,75	0
4	MPO	K	202	13/13	0.82	0.18	52,58,91,93	0
2	TLA	E	201	10/10	0.84	0.31	29,45,52,70	0
2	TLA	A	201	10/10	0.86	0.26	32,48,61,65	0
2	TLA	H	201	10/10	0.86	0.29	32,48,52,71	0
2	TLA	I	201	10/10	0.86	0.23	26,42,49,61	0
2	TLA	F	201	10/10	0.87	0.26	27,44,48,60	0
2	TLA	J	201	10/10	0.87	0.26	26,38,51,60	0
2	TLA	L	201	10/10	0.87	0.25	24,42,53,71	0
2	TLA	C	201	10/10	0.88	0.24	27,45,52,67	0
2	TLA	B	201	10/10	0.88	0.23	26,37,47,65	0
3	GOL	B	202	6/6	0.90	0.23	38,45,48,66	0
2	TLA	K	201	10/10	0.91	0.20	28,42,52,68	0
2	TLA	D	201	10/10	0.91	0.18	28,43,51,63	0

6.5 Other polymers (i)

There are no such residues in this entry.