wwPDB X-ray Structure Validation Summary Report (i)

Aug 26, 2023 – 08:51 PM EDT

PDB ID	:	3EZ4
Title	:	Crystal structure of 3-methyl-2-oxobutanoate hydroxymethyltransferase from Burkholderia pseudomallei
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2008-10-22
Resolution	:	2.10 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

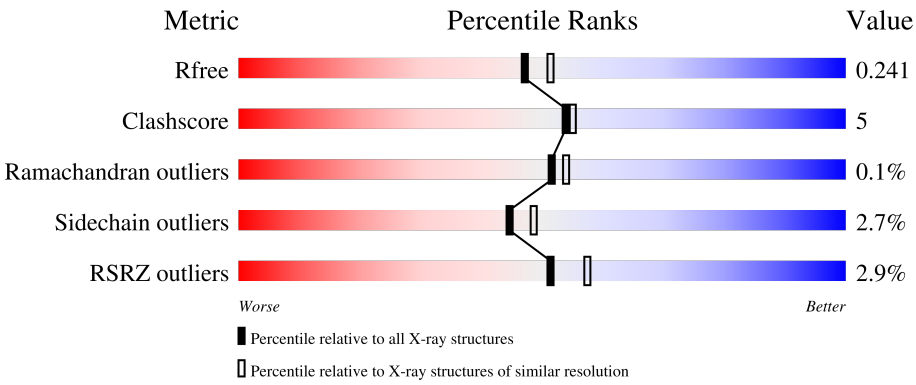
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	269	.% 79% 10% • 10%
1	B	269	2% 78% 11% 10%
1	C	269	2% 79% 10% • 10%
1	D	269	3% 80% 9% 10%
1	E	269	3% 75% 15% 10%

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Mol	Chain	Length	Quality of chain
1	F	269	3% 83% 9% 9%
1	G	269	2% 74% 15% • 10%
1	H	269	2% 79% 10% • 9%
1	I	269	2% 77% 13% • 9%
1	J	269	5% 77% 13% 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 19382 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-methyl-2-oxobutanoate hydroxymethyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	242	1789	1136	311	332	10	0	0	0
1	B	242	1783	1134	309	330	10	0	0	0
1	C	243	1793	1139	311	333	10	0	0	0
1	D	242	1778	1127	309	332	10	0	0	0
1	E	243	1785	1133	309	333	10	0	0	0
1	F	246	1817	1154	317	336	10	0	0	0
1	G	241	1774	1129	305	331	9	0	0	0
1	H	245	1805	1146	311	338	10	0	0	0
1	I	246	1806	1148	312	336	10	0	0	0
1	J	243	1765	1120	305	330	10	0	0	0

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP Q63R49
A	-6	ALA	-	expression tag	UNP Q63R49
A	-5	HIS	-	expression tag	UNP Q63R49
A	-4	HIS	-	expression tag	UNP Q63R49
A	-3	HIS	-	expression tag	UNP Q63R49
A	-2	HIS	-	expression tag	UNP Q63R49
A	-1	HIS	-	expression tag	UNP Q63R49
A	0	HIS	-	expression tag	UNP Q63R49
A	1	MET	-	expression tag	UNP Q63R49

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	MET	-	expression tag	UNP Q63R49
B	-6	ALA	-	expression tag	UNP Q63R49
B	-5	HIS	-	expression tag	UNP Q63R49
B	-4	HIS	-	expression tag	UNP Q63R49
B	-3	HIS	-	expression tag	UNP Q63R49
B	-2	HIS	-	expression tag	UNP Q63R49
B	-1	HIS	-	expression tag	UNP Q63R49
B	0	HIS	-	expression tag	UNP Q63R49
B	1	MET	-	expression tag	UNP Q63R49
C	-7	MET	-	expression tag	UNP Q63R49
C	-6	ALA	-	expression tag	UNP Q63R49
C	-5	HIS	-	expression tag	UNP Q63R49
C	-4	HIS	-	expression tag	UNP Q63R49
C	-3	HIS	-	expression tag	UNP Q63R49
C	-2	HIS	-	expression tag	UNP Q63R49
C	-1	HIS	-	expression tag	UNP Q63R49
C	0	HIS	-	expression tag	UNP Q63R49
C	1	MET	-	expression tag	UNP Q63R49
D	-7	MET	-	expression tag	UNP Q63R49
D	-6	ALA	-	expression tag	UNP Q63R49
D	-5	HIS	-	expression tag	UNP Q63R49
D	-4	HIS	-	expression tag	UNP Q63R49
D	-3	HIS	-	expression tag	UNP Q63R49
D	-2	HIS	-	expression tag	UNP Q63R49
D	-1	HIS	-	expression tag	UNP Q63R49
D	0	HIS	-	expression tag	UNP Q63R49
D	1	MET	-	expression tag	UNP Q63R49
E	-7	MET	-	expression tag	UNP Q63R49
E	-6	ALA	-	expression tag	UNP Q63R49
E	-5	HIS	-	expression tag	UNP Q63R49
E	-4	HIS	-	expression tag	UNP Q63R49
E	-3	HIS	-	expression tag	UNP Q63R49
E	-2	HIS	-	expression tag	UNP Q63R49
E	-1	HIS	-	expression tag	UNP Q63R49
E	0	HIS	-	expression tag	UNP Q63R49
E	1	MET	-	expression tag	UNP Q63R49
F	-7	MET	-	expression tag	UNP Q63R49
F	-6	ALA	-	expression tag	UNP Q63R49
F	-5	HIS	-	expression tag	UNP Q63R49
F	-4	HIS	-	expression tag	UNP Q63R49
F	-3	HIS	-	expression tag	UNP Q63R49
F	-2	HIS	-	expression tag	UNP Q63R49

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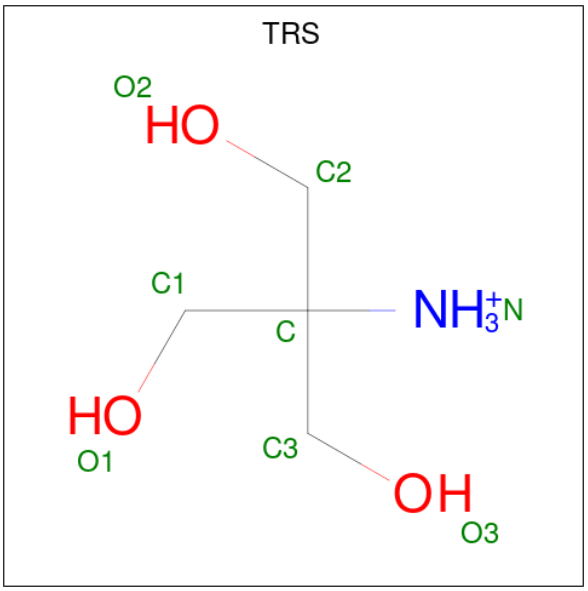
Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	HIS	-	expression tag	UNP Q63R49
F	0	HIS	-	expression tag	UNP Q63R49
F	1	MET	-	expression tag	UNP Q63R49
G	-7	MET	-	expression tag	UNP Q63R49
G	-6	ALA	-	expression tag	UNP Q63R49
G	-5	HIS	-	expression tag	UNP Q63R49
G	-4	HIS	-	expression tag	UNP Q63R49
G	-3	HIS	-	expression tag	UNP Q63R49
G	-2	HIS	-	expression tag	UNP Q63R49
G	-1	HIS	-	expression tag	UNP Q63R49
G	0	HIS	-	expression tag	UNP Q63R49
G	1	MET	-	expression tag	UNP Q63R49
H	-7	MET	-	expression tag	UNP Q63R49
H	-6	ALA	-	expression tag	UNP Q63R49
H	-5	HIS	-	expression tag	UNP Q63R49
H	-4	HIS	-	expression tag	UNP Q63R49
H	-3	HIS	-	expression tag	UNP Q63R49
H	-2	HIS	-	expression tag	UNP Q63R49
H	-1	HIS	-	expression tag	UNP Q63R49
H	0	HIS	-	expression tag	UNP Q63R49
H	1	MET	-	expression tag	UNP Q63R49
I	-7	MET	-	expression tag	UNP Q63R49
I	-6	ALA	-	expression tag	UNP Q63R49
I	-5	HIS	-	expression tag	UNP Q63R49
I	-4	HIS	-	expression tag	UNP Q63R49
I	-3	HIS	-	expression tag	UNP Q63R49
I	-2	HIS	-	expression tag	UNP Q63R49
I	-1	HIS	-	expression tag	UNP Q63R49
I	0	HIS	-	expression tag	UNP Q63R49
I	1	MET	-	expression tag	UNP Q63R49
J	-7	MET	-	expression tag	UNP Q63R49
J	-6	ALA	-	expression tag	UNP Q63R49
J	-5	HIS	-	expression tag	UNP Q63R49
J	-4	HIS	-	expression tag	UNP Q63R49
J	-3	HIS	-	expression tag	UNP Q63R49
J	-2	HIS	-	expression tag	UNP Q63R49
J	-1	HIS	-	expression tag	UNP Q63R49
J	0	HIS	-	expression tag	UNP Q63R49
J	1	MET	-	expression tag	UNP Q63R49

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	E	1	8	4	1	3	0	0
2	F	1	8	4	1	3	0	0
2	G	1	8	4	1	3	0	0
2	H	1	8	4	1	3	0	0
2	I	1	8	4	1	3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	190	190	190	0	0
3	B	126	126	126	0	0
3	C	151	151	151	0	0
3	D	139	139	139	0	0
3	E	127	127	127	0	0
3	F	169	169	169	0	0
3	G	127	127	127	0	0

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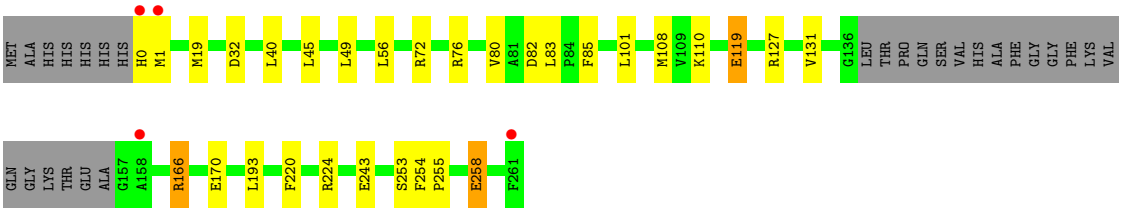
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	H	171	171	171	0	0
			Total	O		
3	I	132	132	132	0	0
			Total	O		
3	J	115	115	115	0	0

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.

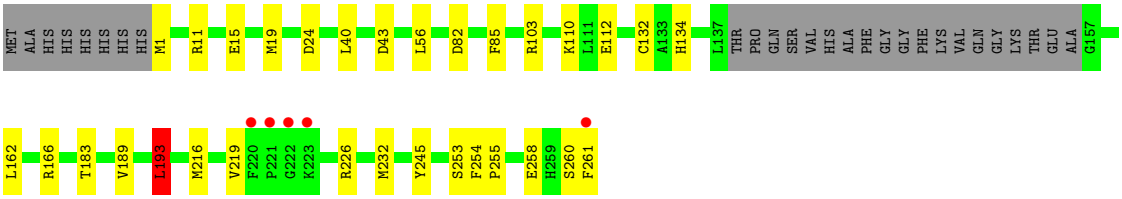
• Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase

Chain A:



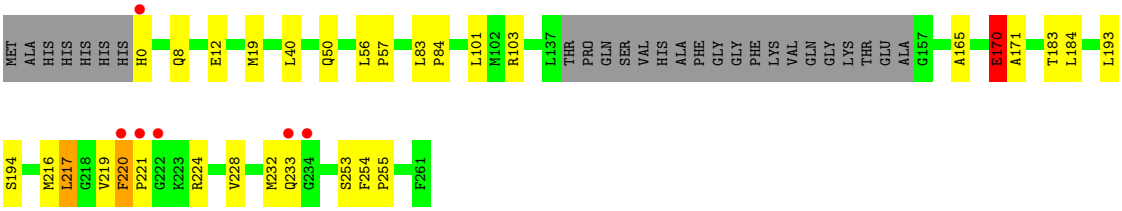
• Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase

Chain B:



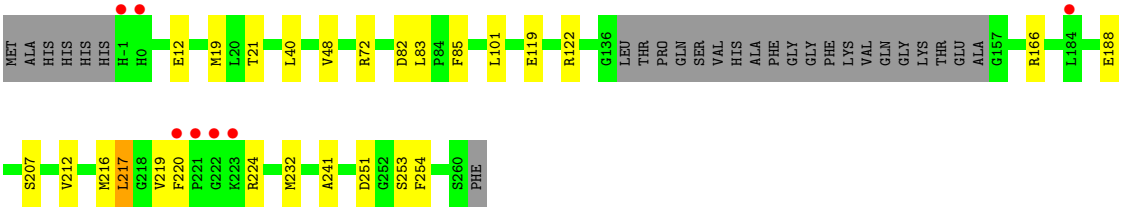
• Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase

Chain C:



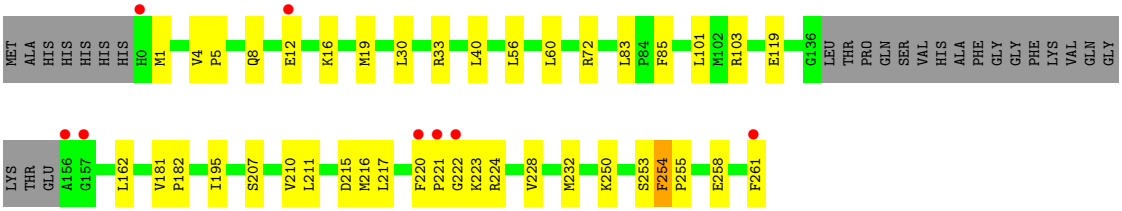
• Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase

Chain D:



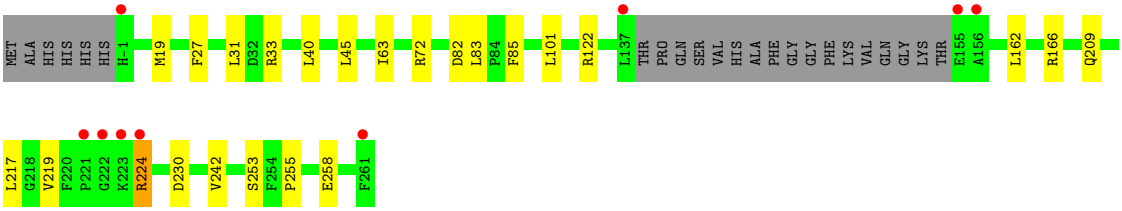
• Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase

Chain E:



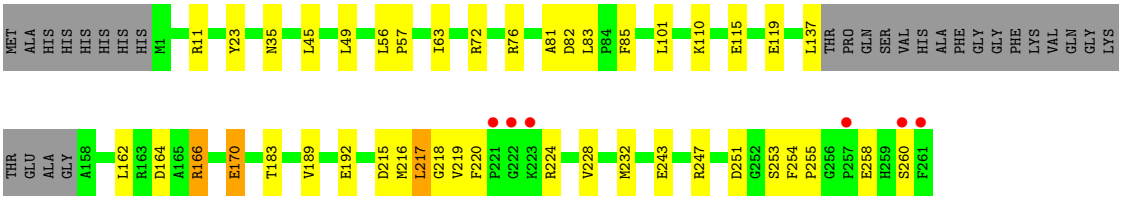
• Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase

Chain F:



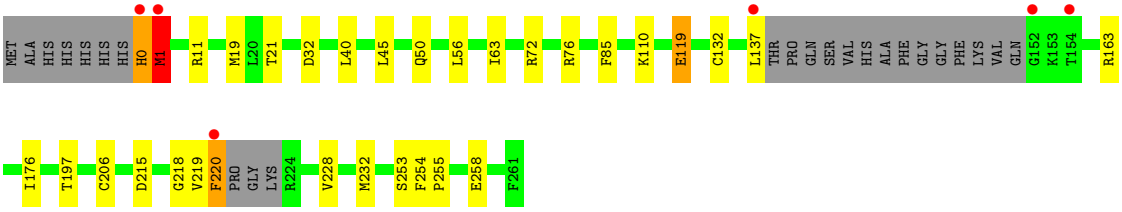
• Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase

Chain G:



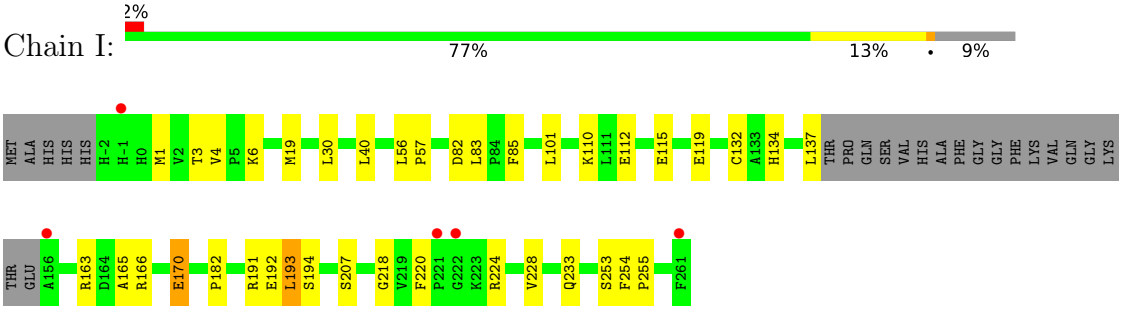
• Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase

Chain H:



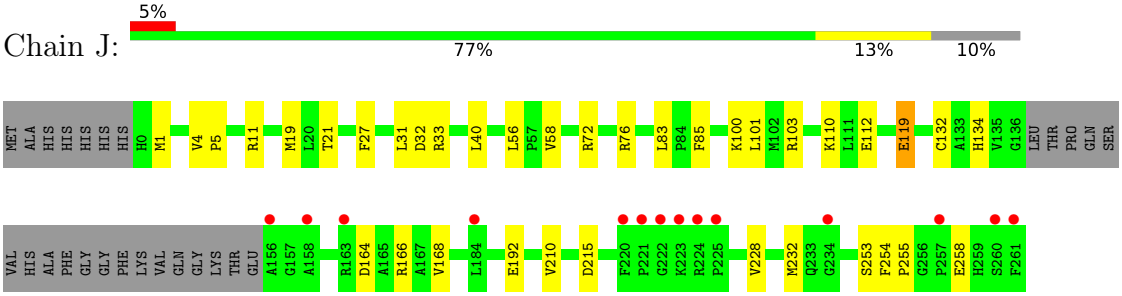
• Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase

Chain I:



• Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	173.78Å 187.56Å 83.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.55 – 2.10 38.54 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.3 (38.55-2.10) 98.3 (38.54-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.80 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.195 , 0.244 0.195 , 0.241	Depositor DCC
R_{free} test set	7886 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	20.5	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	19382	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: TRS

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	1.00	4/1821 (0.2%)	0.88	2/2476 (0.1%)
1	B	0.86	0/1814	0.89	4/2467 (0.2%)
1	C	0.97	1/1825 (0.1%)	0.89	0/2483
1	D	0.84	0/1808	0.88	5/2459 (0.2%)
1	E	0.93	0/1816	0.87	3/2471 (0.1%)
1	F	0.98	1/1850 (0.1%)	0.88	0/2516
1	G	0.89	2/1805 (0.1%)	0.87	2/2457 (0.1%)
1	H	1.00	1/1835 (0.1%)	0.91	3/2494 (0.1%)
1	I	0.96	2/1838 (0.1%)	0.86	0/2501
1	J	0.91	3/1795 (0.2%)	0.87	2/2445 (0.1%)
All	All	0.94	14/18207 (0.1%)	0.88	21/24769 (0.1%)

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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	2
1	I	0	1
1	J	0	1
All	All	0	11

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	170	GLU	CG-CD	9.74	1.66	1.51
1	J	119	GLU	CG-CD	7.34	1.62	1.51
1	I	170	GLU	CB-CG	6.57	1.64	1.52
1	A	243	GLU	CG-CD	6.13	1.61	1.51
1	H	206	CYS	CB-SG	-6.00	1.72	1.82

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	72	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	H	11	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	A	72	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	G	11	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	A	127	ARG	NE-CZ-NH1	6.35	123.47	120.30

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	253	SER	Peptide
1	B	253	SER	Peptide
1	C	253	SER	Peptide
1	D	253	SER	Peptide
1	E	253	SER	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	1789	0	1806	16	0
1	B	1783	0	1806	23	0
1	C	1793	0	1806	18	0
1	D	1778	0	1794	13	0
1	E	1785	0	1795	25	0
1	F	1817	0	1831	16	0
1	G	1774	0	1789	28	0
1	H	1805	0	1816	17	0
1	I	1806	0	1815	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	1765	0	1767	22	0
2	E	8	0	12	0	0
2	F	8	0	12	0	0
2	G	8	0	12	0	0
2	H	8	0	12	0	0
2	I	8	0	12	0	0
3	A	190	0	0	6	0
3	B	126	0	0	2	0
3	C	151	0	0	4	0
3	D	139	0	0	4	0
3	E	127	0	0	3	0
3	F	169	0	0	6	0
3	G	127	0	0	3	0
3	H	171	0	0	4	0
3	I	132	0	0	4	0
3	J	115	0	0	4	0
All	All	19382	0	18085	189	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 5.

The worst 5 of 189 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:G:224:ARG:NH1	1:G:228:VAL:O	2.02	0.92
1:H:119:GLU:OE2	3:H:382:HOH:O	2.00	0.80
1:B:85:PHE:O	1:C:103:ARG:NH1	2.14	0.79
1:D:19:MET:CE	1:D:40:LEU:HD22	2.14	0.78
1:E:33:ARG:HD2	3:E:386:HOH:O	1.86	0.76

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	238/269 (88%)	234 (98%)	4 (2%)	0	100	100
1	B	238/269 (88%)	230 (97%)	8 (3%)	0	100	100
1	C	239/269 (89%)	237 (99%)	2 (1%)	0	100	100
1	D	238/269 (88%)	233 (98%)	5 (2%)	0	100	100
1	E	239/269 (89%)	230 (96%)	8 (3%)	1 (0%)	34	32
1	F	242/269 (90%)	234 (97%)	8 (3%)	0	100	100
1	G	237/269 (88%)	231 (98%)	6 (2%)	0	100	100
1	H	239/269 (89%)	232 (97%)	6 (2%)	1 (0%)	34	32
1	I	242/269 (90%)	234 (97%)	8 (3%)	0	100	100
1	J	239/269 (89%)	233 (98%)	6 (2%)	0	100	100
All	All	2391/2690 (89%)	2328 (97%)	61 (3%)	2 (0%)	51	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	222	GLY
1	H	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	182/204 (89%)	176 (97%)	6 (3%)	38	40
1	B	181/204 (89%)	178 (98%)	3 (2%)	60	67
1	C	182/204 (89%)	174 (96%)	8 (4%)	28	28
1	D	180/204 (88%)	176 (98%)	4 (2%)	52	57
1	E	180/204 (88%)	176 (98%)	4 (2%)	52	57
1	F	184/204 (90%)	181 (98%)	3 (2%)	62	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	180/204 (88%)	173 (96%)	7 (4%)	32	33
1	H	183/204 (90%)	177 (97%)	6 (3%)	38	40
1	I	182/204 (89%)	177 (97%)	5 (3%)	44	48
1	J	176/204 (86%)	173 (98%)	3 (2%)	60	67
All	All	1810/2040 (89%)	1761 (97%)	49 (3%)	44	48

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	85	PHE
1	H	1	MET
1	G	137	LEU
1	G	217	LEU
1	H	119	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	35	ASN
1	J	50	GLN
1	J	35	ASN
1	E	174	GLN
1	H	233	GLN

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)

5 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	TRS	H	262	-	7,7,7	0.28	0	9,9,9	0.78	0
2	TRS	E	262	-	7,7,7	0.31	0	9,9,9	0.98	0
2	TRS	I	262	-	7,7,7	0.25	0	9,9,9	0.69	0
2	TRS	F	262	-	7,7,7	0.37	0	9,9,9	1.32	1 (11%)
2	TRS	G	262	-	7,7,7	0.54	0	9,9,9	1.15	1 (11%)

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	TRS	H	262	-	-	0/9/9/9	-
2	TRS	E	262	-	-	3/9/9/9	-
2	TRS	I	262	-	-	2/9/9/9	-
2	TRS	F	262	-	-	3/9/9/9	-
2	TRS	G	262	-	-	0/9/9/9	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	262	TRS	O2-C2-C	2.39	118.56	111.00
2	G	262	TRS	O3-C3-C	2.05	117.50	111.00

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	262	TRS	N-C-C3-O3
2	E	262	TRS	C2-C-C1-O1
2	F	262	TRS	C3-C-C2-O2
2	E	262	TRS	N-C-C1-O1
2	F	262	TRS	N-C-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	242/269 (89%)	-0.25	4 (1%)	70	74	10, 18, 33, 47	0
1	B	242/269 (89%)	-0.12	5 (2%)	63	68	12, 23, 41, 55	0
1	C	243/269 (90%)	-0.25	6 (2%)	57	62	10, 19, 33, 51	0
1	D	242/269 (89%)	-0.06	7 (2%)	51	57	13, 24, 39, 56	0
1	E	243/269 (90%)	0.03	8 (3%)	46	53	14, 24, 41, 49	0
1	F	246/269 (91%)	-0.14	9 (3%)	41	48	9, 18, 38, 48	0
1	G	241/269 (89%)	-0.14	6 (2%)	57	62	11, 23, 39, 52	0
1	H	245/269 (91%)	-0.23	6 (2%)	59	64	10, 18, 32, 48	0
1	I	246/269 (91%)	-0.31	5 (2%)	65	69	12, 22, 39, 52	0
1	J	243/269 (90%)	0.07	14 (5%)	23	28	11, 23, 43, 57	0
All	All	2433/2690 (90%)	-0.14	70 (2%)	51	57	9, 21, 39, 57	0

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	222	GLY	7.9
1	B	261	PHE	7.4
1	D	222	GLY	5.9
1	F	261	PHE	5.7
1	J	221	PRO	5.6

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, 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	TRS	I	262	8/8	0.86	0.13	27,28,30,31	0
2	TRS	F	262	8/8	0.87	0.11	25,27,28,31	0
2	TRS	E	262	8/8	0.90	0.11	26,28,29,30	0
2	TRS	H	262	8/8	0.92	0.10	27,30,30,31	0
2	TRS	G	262	8/8	0.92	0.11	27,28,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.