Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 08:27 PM BST

PDB ID	:	6OVT
Title	:	Crystal Structure of IlvD from Mycobacterium tuberculosis
Authors	:	Almo, S.C.; Grove, T.L.; Bonanno, J.B.; Baker, E.N.; Bashiri, G.
Deposited on	:	2019-05-08
Resolution	:	1.88 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:

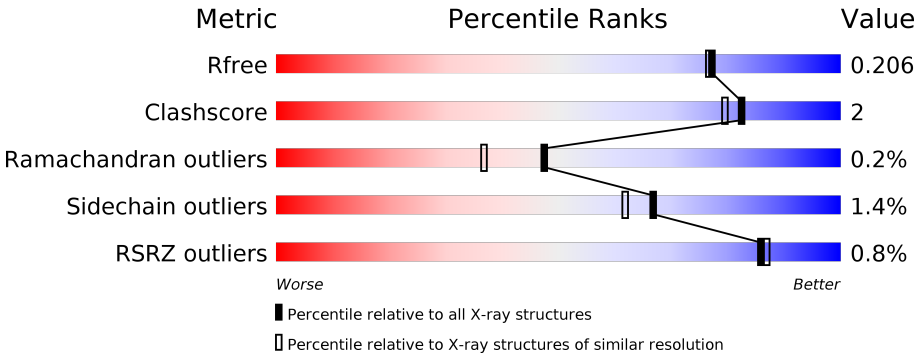
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 1.88 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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	600	87% 7% 6%
1	B	600	% 85% 7% 8%
1	C	600	% 85% 7% • 7%
1	D	600	% 88% 6% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17653 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 Dihydroxy-acid dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	562	Total	C	N	O	S	0	7	0
			4097	2551	727	794	25			
1	B	555	Total	C	N	O	S	0	3	0
			4041	2516	722	777	26			
1	C	558	Total	C	N	O	S	0	10	0
			4098	2551	731	791	25			
1	D	560	Total	C	N	O	S	0	10	0
			4109	2557	732	794	26			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP A0A0E8UWV6
A	-23	SER	-	expression tag	UNP A0A0E8UWV6
A	-22	TYR	-	expression tag	UNP A0A0E8UWV6
A	-21	TYR	-	expression tag	UNP A0A0E8UWV6
A	-20	HIS	-	expression tag	UNP A0A0E8UWV6
A	-19	HIS	-	expression tag	UNP A0A0E8UWV6
A	-18	HIS	-	expression tag	UNP A0A0E8UWV6
A	-17	HIS	-	expression tag	UNP A0A0E8UWV6
A	-16	HIS	-	expression tag	UNP A0A0E8UWV6
A	-15	HIS	-	expression tag	UNP A0A0E8UWV6
A	-14	ASP	-	expression tag	UNP A0A0E8UWV6
A	-13	TYR	-	expression tag	UNP A0A0E8UWV6
A	-12	ASP	-	expression tag	UNP A0A0E8UWV6
A	-11	ILE	-	expression tag	UNP A0A0E8UWV6
A	-10	PRO	-	expression tag	UNP A0A0E8UWV6
A	-9	THR	-	expression tag	UNP A0A0E8UWV6
A	-8	THR	-	expression tag	UNP A0A0E8UWV6
A	-7	GLU	-	expression tag	UNP A0A0E8UWV6
A	-6	ASN	-	expression tag	UNP A0A0E8UWV6
A	-5	LEU	-	expression tag	UNP A0A0E8UWV6
A	-4	TYR	-	expression tag	UNP A0A0E8UWV6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	PHE	-	expression tag	UNP A0A0E8UWV6
A	-2	GLN	-	expression tag	UNP A0A0E8UWV6
A	-1	GLY	-	expression tag	UNP A0A0E8UWV6
A	0	ALA	-	expression tag	UNP A0A0E8UWV6
B	-24	MET	-	initiating methionine	UNP A0A0E8UWV6
B	-23	SER	-	expression tag	UNP A0A0E8UWV6
B	-22	TYR	-	expression tag	UNP A0A0E8UWV6
B	-21	TYR	-	expression tag	UNP A0A0E8UWV6
B	-20	HIS	-	expression tag	UNP A0A0E8UWV6
B	-19	HIS	-	expression tag	UNP A0A0E8UWV6
B	-18	HIS	-	expression tag	UNP A0A0E8UWV6
B	-17	HIS	-	expression tag	UNP A0A0E8UWV6
B	-16	HIS	-	expression tag	UNP A0A0E8UWV6
B	-15	HIS	-	expression tag	UNP A0A0E8UWV6
B	-14	ASP	-	expression tag	UNP A0A0E8UWV6
B	-13	TYR	-	expression tag	UNP A0A0E8UWV6
B	-12	ASP	-	expression tag	UNP A0A0E8UWV6
B	-11	ILE	-	expression tag	UNP A0A0E8UWV6
B	-10	PRO	-	expression tag	UNP A0A0E8UWV6
B	-9	THR	-	expression tag	UNP A0A0E8UWV6
B	-8	THR	-	expression tag	UNP A0A0E8UWV6
B	-7	GLU	-	expression tag	UNP A0A0E8UWV6
B	-6	ASN	-	expression tag	UNP A0A0E8UWV6
B	-5	LEU	-	expression tag	UNP A0A0E8UWV6
B	-4	TYR	-	expression tag	UNP A0A0E8UWV6
B	-3	PHE	-	expression tag	UNP A0A0E8UWV6
B	-2	GLN	-	expression tag	UNP A0A0E8UWV6
B	-1	GLY	-	expression tag	UNP A0A0E8UWV6
B	0	ALA	-	expression tag	UNP A0A0E8UWV6
C	-24	MET	-	initiating methionine	UNP A0A0E8UWV6
C	-23	SER	-	expression tag	UNP A0A0E8UWV6
C	-22	TYR	-	expression tag	UNP A0A0E8UWV6
C	-21	TYR	-	expression tag	UNP A0A0E8UWV6
C	-20	HIS	-	expression tag	UNP A0A0E8UWV6
C	-19	HIS	-	expression tag	UNP A0A0E8UWV6
C	-18	HIS	-	expression tag	UNP A0A0E8UWV6
C	-17	HIS	-	expression tag	UNP A0A0E8UWV6
C	-16	HIS	-	expression tag	UNP A0A0E8UWV6
C	-15	HIS	-	expression tag	UNP A0A0E8UWV6
C	-14	ASP	-	expression tag	UNP A0A0E8UWV6
C	-13	TYR	-	expression tag	UNP A0A0E8UWV6
C	-12	ASP	-	expression tag	UNP A0A0E8UWV6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	ILE	-	expression tag	UNP A0A0E8UWV6
C	-10	PRO	-	expression tag	UNP A0A0E8UWV6
C	-9	THR	-	expression tag	UNP A0A0E8UWV6
C	-8	THR	-	expression tag	UNP A0A0E8UWV6
C	-7	GLU	-	expression tag	UNP A0A0E8UWV6
C	-6	ASN	-	expression tag	UNP A0A0E8UWV6
C	-5	LEU	-	expression tag	UNP A0A0E8UWV6
C	-4	TYR	-	expression tag	UNP A0A0E8UWV6
C	-3	PHE	-	expression tag	UNP A0A0E8UWV6
C	-2	GLN	-	expression tag	UNP A0A0E8UWV6
C	-1	GLY	-	expression tag	UNP A0A0E8UWV6
C	0	ALA	-	expression tag	UNP A0A0E8UWV6
D	-24	MET	-	initiating methionine	UNP A0A0E8UWV6
D	-23	SER	-	expression tag	UNP A0A0E8UWV6
D	-22	TYR	-	expression tag	UNP A0A0E8UWV6
D	-21	TYR	-	expression tag	UNP A0A0E8UWV6
D	-20	HIS	-	expression tag	UNP A0A0E8UWV6
D	-19	HIS	-	expression tag	UNP A0A0E8UWV6
D	-18	HIS	-	expression tag	UNP A0A0E8UWV6
D	-17	HIS	-	expression tag	UNP A0A0E8UWV6
D	-16	HIS	-	expression tag	UNP A0A0E8UWV6
D	-15	HIS	-	expression tag	UNP A0A0E8UWV6
D	-14	ASP	-	expression tag	UNP A0A0E8UWV6
D	-13	TYR	-	expression tag	UNP A0A0E8UWV6
D	-12	ASP	-	expression tag	UNP A0A0E8UWV6
D	-11	ILE	-	expression tag	UNP A0A0E8UWV6
D	-10	PRO	-	expression tag	UNP A0A0E8UWV6
D	-9	THR	-	expression tag	UNP A0A0E8UWV6
D	-8	THR	-	expression tag	UNP A0A0E8UWV6
D	-7	GLU	-	expression tag	UNP A0A0E8UWV6
D	-6	ASN	-	expression tag	UNP A0A0E8UWV6
D	-5	LEU	-	expression tag	UNP A0A0E8UWV6
D	-4	TYR	-	expression tag	UNP A0A0E8UWV6
D	-3	PHE	-	expression tag	UNP A0A0E8UWV6
D	-2	GLN	-	expression tag	UNP A0A0E8UWV6
D	-1	GLY	-	expression tag	UNP A0A0E8UWV6
D	0	ALA	-	expression tag	UNP A0A0E8UWV6

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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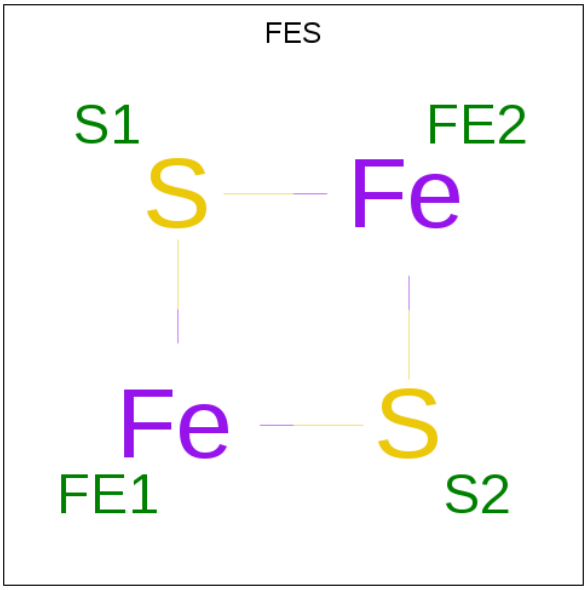
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf

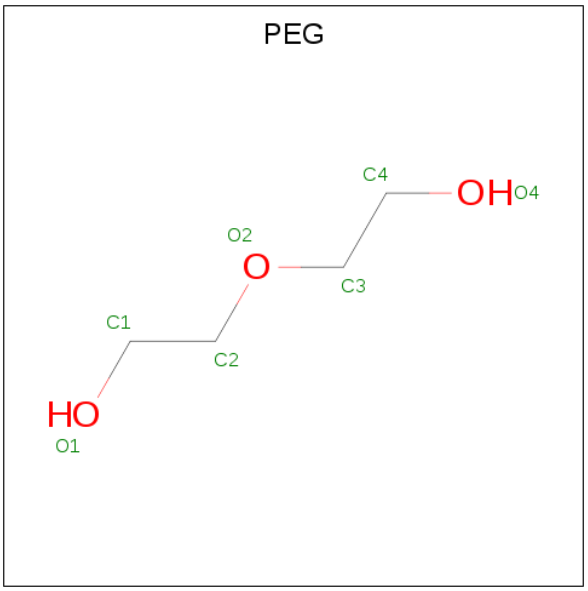
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Mg 3 3	0	0
2	A	3	Total Mg 3 3	0	0
2	D	3	Total Mg 3 3	0	0
2	C	3	Total Mg 3 3	0	0

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 4 2 2	0	0
3	B	1	Total Fe S 4 2 2	0	0
3	C	1	Total Fe S 4 2 2	0	0
3	D	1	Total Fe S 4 2 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total Na 1 1	0	0

- Molecule 6 is water.

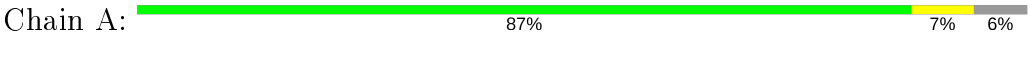
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	382	Total O 382 382	0	0
6	B	256	Total O 256 256	0	0
6	C	306	Total O 306 306	0	0
6	D	314	Total O 314 314	0	0

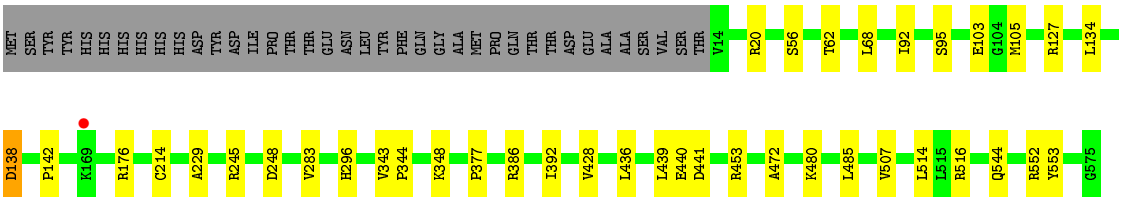
3 Residue-property plots (i)

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: Dihydroxy-acid dehydratase

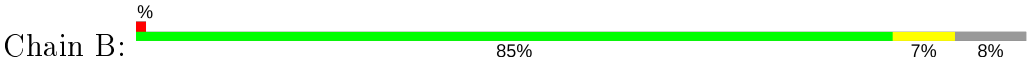
Chain A:

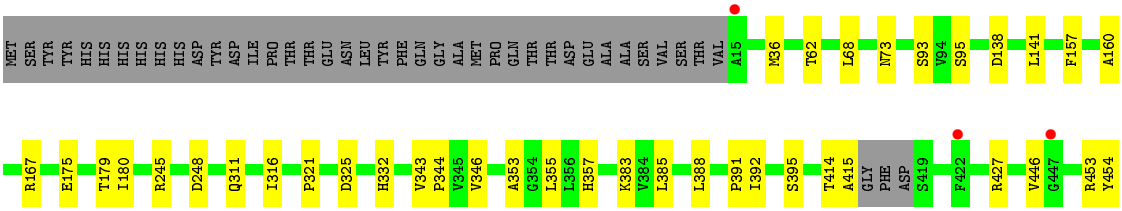




- Molecule 1: Dihydroxy-acid dehydratase

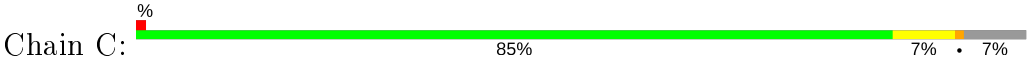
Chain B:

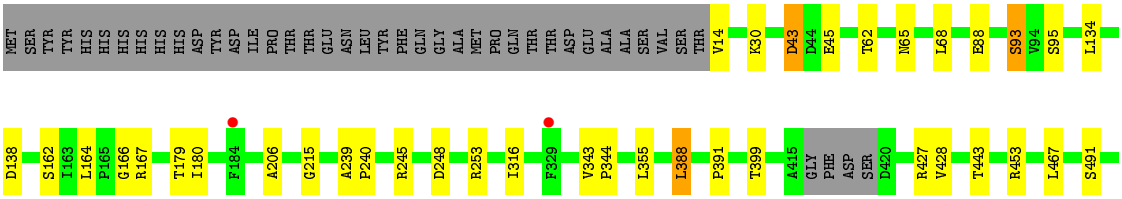




- Molecule 1: Dihydroxy-acid dehydratase

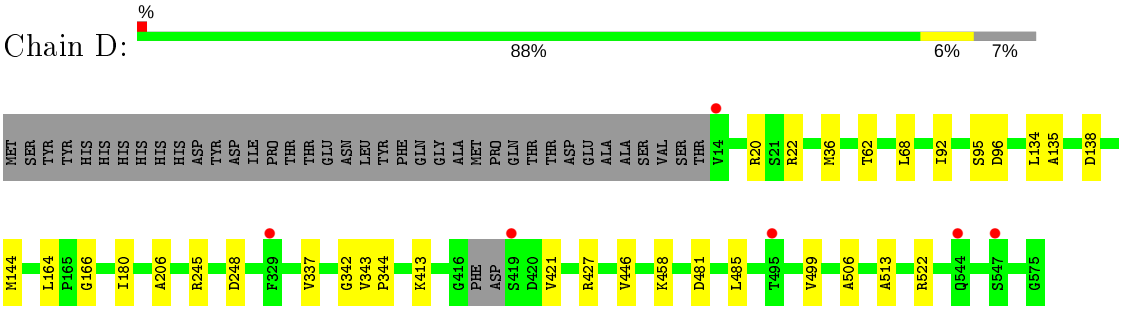
Chain C:





• Molecule 1: Dihydroxy-acid dehydratase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	88.41Å 88.41Å 483.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	80.55 – 1.88 80.55 – 1.88	Depositor EDS
% Data completeness (in resolution range)	100.0 (80.55-1.88) 100.0 (80.55-1.88)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.95 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.160 , 0.201 0.168 , 0.206	Depositor DCC
R_{free} test set	8430 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	26.7	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.059 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	17653	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 3.35% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MG, PEG, FES, KCX

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	0.78	0/4163	0.84	4/5643 (0.1%)
1	B	0.74	0/4092	0.80	1/5541 (0.0%)
1	C	0.75	0/4165	0.83	1/5641 (0.0%)
1	D	0.75	0/4176	0.81	1/5657 (0.0%)
All	All	0.75	0/16596	0.82	7/22482 (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	A	0	2
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	20	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	A	20	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	A	127	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	127	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	D	427	ARG	CG-CD-NE	-5.26	100.76	111.80
1	C	253	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	B	575	GLY	CA-C-O	-5.10	111.42	120.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	CYS	Peptide
1	A	92	ILE	Peptide
1	D	92	ILE	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	4097	0	4112	17	0
1	B	4041	0	4057	25	0
1	C	4098	0	4127	26	0
1	D	4109	0	4132	19	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	7	0	10	0	0
4	B	7	0	10	3	0
4	C	7	0	10	2	0
5	D	1	0	0	0	0
6	A	382	0	0	3	0
6	B	256	0	0	2	0
6	C	306	0	0	4	0
6	D	314	0	0	4	0
All	All	17653	0	16458	82	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 (82) 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:427[A]:ARG:HE	1:C:443:THR:HG22	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:ASP:HB3	1:C:45:GLU:OE2	2.01	0.61
1:D:446:VAL:HG13	1:D:481:ASP:HB3	1.84	0.60
1:D:68:LEU:HD22	1:D:134:LEU:HB3	1.85	0.59
1:D:20[A]:ARG:NH2	6:D:702:HOH:O	2.16	0.58
1:B:36[A]:MET:SD	1:D:180:ILE:HD11	2.44	0.57
1:A:516:ARG:HA	6:A:810:HOH:O	2.04	0.57
1:A:68:LEU:HD22	1:A:134:LEU:HB3	1.87	0.55
1:A:56[A]:SER:HB3	6:A:716:HOH:O	2.05	0.55
1:A:62:THR:HB	1:A:95:SER:HB2	1.90	0.54
1:B:357:HIS:CE1	4:B:603:PEG:H11	2.43	0.53
1:A:428:VAL:HG11	1:A:453:ARG:CZ	2.39	0.52
1:C:427[B]:ARG:NH1	6:C:710:HOH:O	2.42	0.52
1:B:316:ILE:HD12	4:B:603:PEG:H42	1.92	0.52
1:C:14:VAL:HG22	6:C:849:HOH:O	2.10	0.52
1:C:388:LEU:O	1:C:391:PRO:HD3	2.10	0.51
1:C:65:ASN:ND2	1:C:93:SER:OG	2.41	0.51
1:D:62:THR:HB	1:D:95:SER:HB2	1.92	0.51
1:A:439:LEU:HD22	1:A:472:ALA:HB1	1.92	0.51
1:B:446:VAL:HG23	1:B:481:ASP:HB3	1.93	0.51
1:C:162[B]:SER:OG	1:C:215:GLY:HA2	2.10	0.51
1:B:36[A]:MET:CG	1:D:180:ILE:HD11	2.42	0.50
1:B:180:ILE:HD11	1:D:36:MET:SD	2.52	0.50
1:D:96:ASP:HB3	6:D:905:HOH:O	2.12	0.49
1:B:179:THR:OG1	1:B:180:ILE:N	2.43	0.49
1:B:62:THR:HB	1:B:95:SER:HB2	1.95	0.49
1:C:316:ILE:HG23	4:C:602:PEG:H22	1.95	0.49
1:C:179:THR:OG1	1:C:180:ILE:N	2.45	0.49
1:C:62:THR:HB	1:C:95:SER:HB2	1.94	0.48
1:C:88:GLU:OE1	6:C:701:HOH:O	2.19	0.48
1:D:135:ALA:HB2	1:D:144[B]:MET:HG3	1.95	0.48
1:B:343:VAL:N	1:B:344:PRO:CD	2.76	0.48
1:C:68:LEU:HD22	1:C:134:LEU:HB3	1.94	0.48
1:A:514:LEU:HA	1:A:544:GLN:HG3	1.96	0.47
1:A:142:PRO:HB3	1:A:296:HIS:HB3	1.95	0.47
1:D:485:LEU:HD23	1:D:499:VAL:HB	1.97	0.47
1:C:427[A]:ARG:HH21	1:C:443:THR:HG21	1.81	0.46
1:C:538:GLU:O	1:C:541:SER:HB3	2.15	0.46
1:D:458:LYS:NZ	6:D:728:HOH:O	2.47	0.46
1:C:527:GLY:O	1:C:529:VAL:HG23	2.16	0.46
1:C:503:ALA:HA	1:C:504:PRO:C	2.35	0.46
1:C:164:LEU:HD13	1:D:164:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:ARG:HB2	6:D:803:HOH:O	2.15	0.46
1:A:138:ASP:O	1:A:142:PRO:HD2	2.16	0.45
1:A:436:LEU:O	1:A:440:GLU:HG2	2.17	0.44
1:D:166:GLY:HA3	1:D:206:ALA:O	2.17	0.44
1:C:355:LEU:C	4:C:602:PEG:H41	2.38	0.44
1:B:167:ARG:NH1	1:B:175:GLU:OE1	2.51	0.44
1:B:353:ALA:HB2	1:B:388:LEU:HD13	1.99	0.44
1:B:325:ASP:HB2	1:B:392:ILE:HD11	2.00	0.44
1:B:346:VAL:HG23	1:B:385:LEU:HD13	2.00	0.44
1:C:343:VAL:N	1:C:344:PRO:CD	2.81	0.44
1:A:229:ALA:HB2	1:A:283:VAL:HG21	2.01	0.43
1:B:414:THR:O	1:B:415:ALA:C	2.56	0.43
1:C:399:THR:HG23	1:C:528[B]:ARG:HH11	1.84	0.43
1:A:343:VAL:N	1:A:344:PRO:CD	2.82	0.43
1:B:332:HIS:NE2	1:B:383:LYS:HE2	2.34	0.43
1:B:68:LEU:HD21	1:B:160:ALA:HB2	2.02	0.42
1:B:73:ASN:ND2	6:B:703:HOH:O	2.26	0.42
1:B:503:ALA:HA	1:B:504:PRO:C	2.40	0.42
1:D:421:VAL:HG11	1:D:522:ARG:NH1	2.35	0.42
1:B:355:LEU:C	4:B:603:PEG:H21	2.41	0.41
1:C:166:GLY:HA3	1:C:206:ALA:O	2.19	0.41
1:D:337:VAL:HG12	1:D:342:GLY:HA2	2.02	0.41
1:A:386:ARG:HG3	1:A:392:ILE:HG13	2.02	0.41
1:C:239:ALA:N	1:C:240:PRO:CD	2.84	0.41
1:B:427:ARG:NH2	6:B:725:HOH:O	2.52	0.41
1:A:348:LYS:HD2	1:A:377:PRO:HD2	2.02	0.41
1:B:141:LEU:HG	1:B:157:PHE:CZ	2.55	0.41
1:B:141:LEU:HG	1:B:157:PHE:HZ	1.85	0.41
1:C:164:LEU:HD13	1:D:164:LEU:CD1	2.51	0.41
1:A:103:GLU:HG2	1:A:552:ARG:NH2	2.35	0.41
1:D:343:VAL:N	1:D:344:PRO:CD	2.84	0.41
1:D:506:ALA:HA	1:D:513:ALA:HB2	2.01	0.41
1:B:311:GLN:H	1:B:311:GLN:CD	2.25	0.40
1:C:428:VAL:HG11	1:C:453:ARG:CZ	2.50	0.40
1:A:553:TYR:N	6:A:736:HOH:O	2.53	0.40
1:A:441:ASP:OD1	1:A:441:ASP:C	2.60	0.40
1:B:321:PRO:HB2	1:B:391:PRO:HB3	2.04	0.40
1:B:453:ARG:HG3	1:B:454:TYR:CD2	2.57	0.40
1:C:506:ALA:HA	1:C:513:ALA:HB2	2.04	0.40
1:C:388:LEU:HD13	6:C:798:HOH:O	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	566/600 (94%)	556 (98%)	9 (2%)	1 (0%)	47	37
1	B	551/600 (92%)	537 (98%)	13 (2%)	1 (0%)	47	37
1	C	563/600 (94%)	552 (98%)	10 (2%)	1 (0%)	47	37
1	D	565/600 (94%)	553 (98%)	11 (2%)	1 (0%)	47	37
All	All	2245/2400 (94%)	2198 (98%)	43 (2%)	4 (0%)	47	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	138	ASP
1	C	138	ASP
1	D	138	ASP
1	A	138	ASP

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	424/451 (94%)	417 (98%)	7 (2%)	60	54
1	B	415/451 (92%)	411 (99%)	4 (1%)	76	73
1	C	424/451 (94%)	414 (98%)	10 (2%)	49	39
1	D	425/451 (94%)	422 (99%)	3 (1%)	84	83
All	All	1688/1804 (94%)	1664 (99%)	24 (1%)	67	62

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	MET
1	A	176	ARG
1	A	245	ARG
1	A	248	ASP
1	A	480	LYS
1	A	485	LEU
1	A	507	VAL
1	B	93	SER
1	B	245	ARG
1	B	248	ASP
1	B	395	SER
1	C	30	LYS
1	C	43	ASP
1	C	93	SER
1	C	167	ARG
1	C	245	ARG
1	C	248	ASP
1	C	388	LEU
1	C	467	LEU
1	C	491	SER
1	C	541	SER
1	D	245	ARG
1	D	248	ASP
1	D	413	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	390	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	KCX	C	139	1,2	7,11,12	0.61	0	4,12,14	0.67	0
1	KCX	B	139	1,2	7,11,12	0.57	0	4,12,14	0.72	0
1	KCX	D	139	1,2	7,11,12	0.56	0	4,12,14	0.35	0
1	KCX	A	139	1,2	7,11,12	0.44	0	4,12,14	0.33	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
1	KCX	C	139	1,2	-	0/7/10/12	-
1	KCX	B	139	1,2	-	0/7/10/12	-
1	KCX	D	139	1,2	-	0/7/10/12	-
1	KCX	A	139	1,2	-	0/7/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 13 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
3	FES	A	602	1,6	0,4,4	0.00	-	-		
3	FES	C	601	1,6	0,4,4	0.00	-	-		
4	PEG	C	602	-	6,6,6	0.24	0	5,5,5	0.18	0
4	PEG	A	605	-	6,6,6	0.32	0	5,5,5	0.13	0
3	FES	B	602	1,6	0,4,4	0.00	-	-		
4	PEG	B	603	-	6,6,6	0.25	0	5,5,5	0.16	0
3	FES	D	603	1,6	0,4,4	0.00	-	-		

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
3	FES	A	602	1,6	-	-	0/1/1/1
3	FES	C	601	1,6	-	-	0/1/1/1
4	PEG	C	602	-	-	1/4/4/4	-
4	PEG	A	605	-	-	2/4/4/4	-
3	FES	B	602	1,6	-	-	0/1/1/1
4	PEG	B	603	-	-	3/4/4/4	-
3	FES	D	603	1,6	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	602	PEG	O2-C3-C4-O4
4	B	603	PEG	O1-C1-C2-O2
4	A	605	PEG	O1-C1-C2-O2
4	B	603	PEG	C4-C3-O2-C2
4	A	605	PEG	O2-C3-C4-O4
4	B	603	PEG	O2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	602	PEG	2	0
4	B	603	PEG	3	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	561/600 (93%)	-0.55	1 (0%)	95	95	17, 25, 46, 73	0
1	B	554/600 (92%)	-0.37	4 (0%)	87	88	20, 34, 62, 81	0
1	C	557/600 (92%)	-0.37	7 (1%)	77	79	17, 29, 68, 94	0
1	D	559/600 (93%)	-0.38	6 (1%)	80	82	18, 31, 62, 107	0
All	All	2231/2400 (92%)	-0.42	18 (0%)	86	87	17, 30, 60, 107	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	419	SER	3.4
1	B	15	ALA	2.8
1	C	550	PRO	2.5
1	C	526	ALA	2.4
1	C	184	PHE	2.4
1	D	14	VAL	2.4
1	D	329	PHE	2.4
1	B	447	GLY	2.4
1	D	547	SER	2.4
1	C	539	PHE	2.4
1	D	544	GLN	2.2
1	C	329	PHE	2.2
1	B	575	GLY	2.1
1	A	169	LYS	2.1
1	C	544	GLN	2.1
1	B	422	PHE	2.1
1	C	533	LEU	2.0
1	D	495	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	KCX	C	139	12/13	0.90	0.11	22,23,30,32	0
1	KCX	B	139	12/13	0.94	0.09	27,30,34,35	0
1	KCX	D	139	12/13	0.94	0.09	24,27,34,35	0
1	KCX	A	139	12/13	0.97	0.07	18,19,23,23	0

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
5	NA	D	605	1/1	0.69	0.23	62,62,62,62	0
2	MG	D	604	1/1	0.83	0.10	49,49,49,49	0
4	PEG	B	603	7/7	0.83	0.11	56,56,58,59	0
4	PEG	C	602	7/7	0.84	0.12	48,51,54,56	0
2	MG	D	602	1/1	0.85	0.10	48,48,48,48	0
4	PEG	A	605	7/7	0.87	0.11	38,46,47,49	0
2	MG	B	605	1/1	0.88	0.06	48,48,48,48	0
2	MG	A	603	1/1	0.90	0.05	50,50,50,50	0
2	MG	B	604	1/1	0.94	0.06	50,50,50,50	0
2	MG	B	601	1/1	0.95	0.05	36,36,36,36	0
2	MG	D	601	1/1	0.96	0.09	40,40,40,40	0
2	MG	A	604	1/1	0.96	0.05	42,42,42,42	0
2	MG	C	604	1/1	0.96	0.04	41,41,41,41	0
2	MG	A	601	1/1	0.97	0.05	23,23,23,23	0
2	MG	C	605	1/1	0.98	0.07	39,39,39,39	0
2	MG	C	603	1/1	0.98	0.11	32,32,32,32	0
3	FES	C	601	4/4	0.99	0.05	24,26,29,30	0
3	FES	D	603	4/4	0.99	0.07	23,25,25,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FES	B	602	4/4	0.99	0.06	28,28,30,31	0
3	FES	A	602	4/4	1.00	0.06	21,22,23,24	0

6.5 Other polymers (i)

There are no such residues in this entry.