



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 10:16 am BST

PDB ID : 4TQT
Title : Crystal structure of Dihydropyrimidinase from Brucella suis
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2014-06-12
Resolution : 2.15 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 : 2.11
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

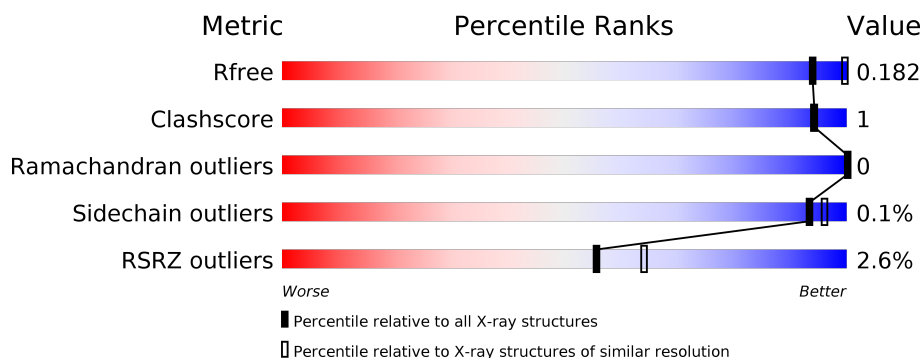
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	497	<div> <div>5%</div> <div> <div></div> <div>92%</div> <div></div> </div> <div></div> </div>
1	B	497	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div></div> </div> <div></div> </div>
1	C	497	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div></div> </div> <div></div> </div>
1	D	497	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div></div> </div> <div></div> </div>
1	E	497	<div> <div>%</div> <div> <div></div> <div>92%</div> <div></div> </div> <div></div> </div>
1	F	497	<div> <div>3%</div> <div> <div></div> <div>94%</div> <div></div> </div> <div></div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23274 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 D-hydantoinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	0	0
			3633	2274	643	696	20			
1	B	477	Total	C	N	O	S	0	4	0
			3674	2305	649	700	20			
1	C	476	Total	C	N	O	S	0	2	0
			3628	2275	638	695	20			
1	D	481	Total	C	N	O	S	0	4	0
			3689	2314	650	705	20			
1	E	477	Total	C	N	O	S	0	4	0
			3665	2301	645	699	20			
1	F	481	Total	C	N	O	S	0	3	0
			3639	2283	637	698	21			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP Q8G2P0
A	-6	ALA	-	expression tag	UNP Q8G2P0
A	-5	HIS	-	expression tag	UNP Q8G2P0
A	-4	HIS	-	expression tag	UNP Q8G2P0
A	-3	HIS	-	expression tag	UNP Q8G2P0
A	-2	HIS	-	expression tag	UNP Q8G2P0
A	-1	HIS	-	expression tag	UNP Q8G2P0
A	0	HIS	-	expression tag	UNP Q8G2P0
B	-7	MET	-	expression tag	UNP Q8G2P0
B	-6	ALA	-	expression tag	UNP Q8G2P0
B	-5	HIS	-	expression tag	UNP Q8G2P0
B	-4	HIS	-	expression tag	UNP Q8G2P0
B	-3	HIS	-	expression tag	UNP Q8G2P0
B	-2	HIS	-	expression tag	UNP Q8G2P0
B	-1	HIS	-	expression tag	UNP Q8G2P0
B	0	HIS	-	expression tag	UNP Q8G2P0
C	-7	MET	-	expression tag	UNP Q8G2P0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	ALA	-	expression tag	UNP Q8G2P0
C	-5	HIS	-	expression tag	UNP Q8G2P0
C	-4	HIS	-	expression tag	UNP Q8G2P0
C	-3	HIS	-	expression tag	UNP Q8G2P0
C	-2	HIS	-	expression tag	UNP Q8G2P0
C	-1	HIS	-	expression tag	UNP Q8G2P0
C	0	HIS	-	expression tag	UNP Q8G2P0
D	-7	MET	-	expression tag	UNP Q8G2P0
D	-6	ALA	-	expression tag	UNP Q8G2P0
D	-5	HIS	-	expression tag	UNP Q8G2P0
D	-4	HIS	-	expression tag	UNP Q8G2P0
D	-3	HIS	-	expression tag	UNP Q8G2P0
D	-2	HIS	-	expression tag	UNP Q8G2P0
D	-1	HIS	-	expression tag	UNP Q8G2P0
D	0	HIS	-	expression tag	UNP Q8G2P0
E	-7	MET	-	expression tag	UNP Q8G2P0
E	-6	ALA	-	expression tag	UNP Q8G2P0
E	-5	HIS	-	expression tag	UNP Q8G2P0
E	-4	HIS	-	expression tag	UNP Q8G2P0
E	-3	HIS	-	expression tag	UNP Q8G2P0
E	-2	HIS	-	expression tag	UNP Q8G2P0
E	-1	HIS	-	expression tag	UNP Q8G2P0
E	0	HIS	-	expression tag	UNP Q8G2P0
F	-7	MET	-	expression tag	UNP Q8G2P0
F	-6	ALA	-	expression tag	UNP Q8G2P0
F	-5	HIS	-	expression tag	UNP Q8G2P0
F	-4	HIS	-	expression tag	UNP Q8G2P0
F	-3	HIS	-	expression tag	UNP Q8G2P0
F	-2	HIS	-	expression tag	UNP Q8G2P0
F	-1	HIS	-	expression tag	UNP Q8G2P0
F	0	HIS	-	expression tag	UNP Q8G2P0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

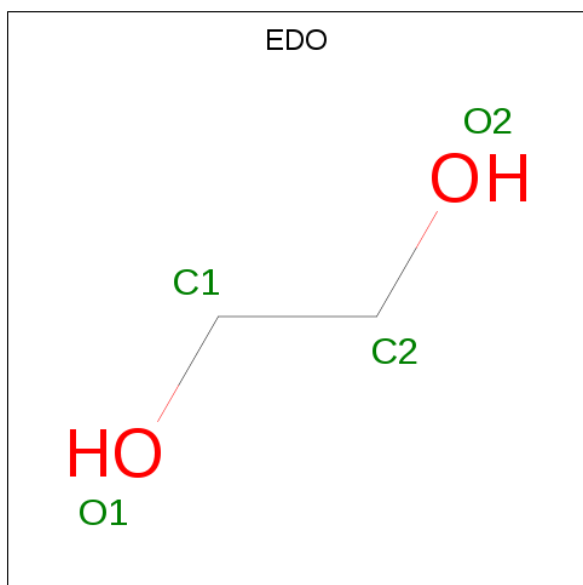
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Zn 2	0	0
2	F	2	Total 2	Zn 2	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	198	Total O 198 198	0	0
4	B	244	Total O 244 244	0	0
4	C	195	Total O 195 195	0	0
4	D	208	Total O 208 208	0	0

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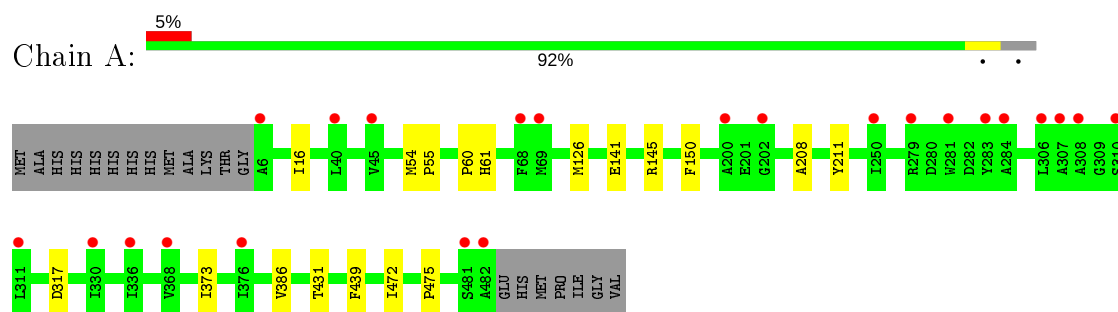
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	220	Total 220	O 220	0	0
4	F	173	Total 173	O 173	0	0

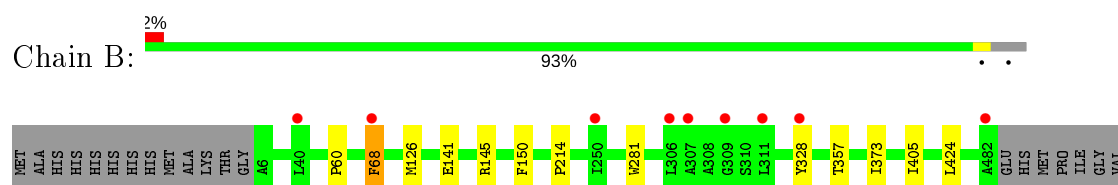
3 Residue-property plots [i](#)

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.

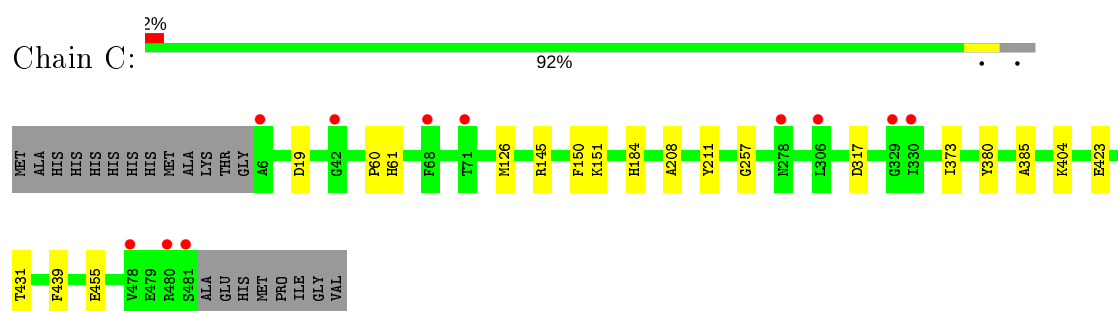
• Molecule 1: D-hydantoinase



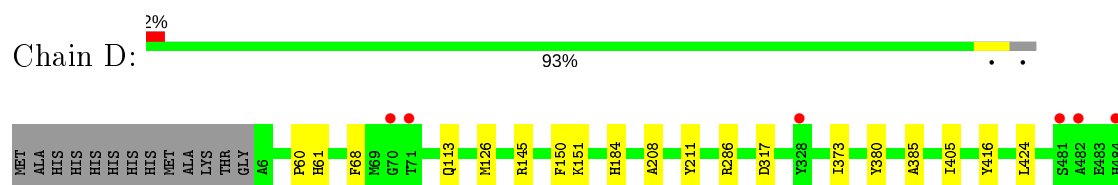
• Molecule 1: D-hydantoinase



• Molecule 1: D-hydantoinase

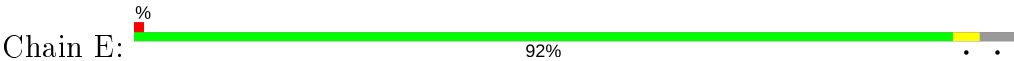


• Molecule 1: D-hydantoinase

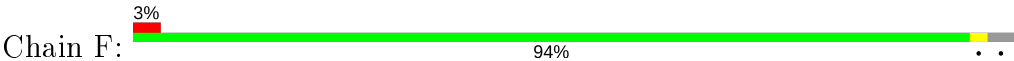




● Molecule 1: D-hydantoinase



● Molecule 1: D-hydantoinase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	156.69Å 88.83Å 221.24Å 90.00° 91.17° 90.00°	Depositor
Resolution (Å)	44.24 – 2.15 45.02 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.24-2.15) 99.9 (45.02-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.16Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.135 , 0.182 0.141 , 0.182	Depositor DCC
R_{free} test set	8376 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.010 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.011 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.013 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.016 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.012 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	23274	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, EDO, 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	0.37	0/3696	0.51	0/5013
1	B	0.40	0/3751	0.54	0/5084
1	C	0.37	0/3697	0.50	0/5013
1	D	0.38	0/3767	0.52	0/5111
1	E	0.38	0/3742	0.51	0/5073
1	F	0.34	0/3713	0.49	0/5042
All	All	0.38	0/22366	0.51	0/30336

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	3633	0	3502	11	0
1	B	3674	0	3563	8	0
1	C	3628	0	3507	14	0
1	D	3689	0	3554	11	0
1	E	3665	0	3551	12	0
1	F	3639	0	3483	6	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	20	0	30	0	0
3	B	12	0	18	0	0
3	C	16	0	24	1	0
3	D	16	0	24	1	0
3	E	16	0	24	1	0
3	F	16	0	24	0	0
4	A	198	0	0	1	0
4	B	244	0	0	1	0
4	C	195	0	0	1	0
4	D	208	0	0	1	0
4	E	220	0	0	2	0
4	F	173	0	0	0	0
All	All	23274	0	21304	58	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 1.

All (58) 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:E:60:PRO:HB3	1:E:373:ILE:HG12	1.74	0.68
1:E:19:ASP:OD2	4:E:815:HOH:O	2.13	0.66
1:D:60:PRO:HB3	1:D:373:ILE:HG12	1.80	0.63
1:F:60:PRO:HB3	1:F:373:ILE:HG12	1.82	0.60
1:C:404:LYS:NZ	1:C:423:GLU:OE2	2.30	0.59
1:C:60:PRO:HB3	1:C:373:ILE:HG12	1.83	0.59
1:D:113:GLN:NE2	4:D:601:HOH:O	2.35	0.58
1:B:60:PRO:HB3	1:B:373:ILE:HG12	1.84	0.58
1:F:17:THR:OG1	1:F:19[A]:ASP:OD1	2.23	0.57
1:B:68:PHE:HZ	1:B:328:TYR:HD2	1.51	0.57
1:A:60:PRO:HB3	1:A:373:ILE:HG12	1.85	0.56
1:B:281:TRP:HB3	1:D:486:PRO:HD3	1.86	0.56
1:D:380:TYR:CE1	1:D:385:ALA:HB2	2.42	0.55
1:C:257:GLY:O	3:C:505:EDO:H12	2.09	0.53
1:C:151:KCX:OQ1	1:C:184:HIS:HB2	2.10	0.52
1:E:257:GLY:O	3:E:505:EDO:H12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ARG:HD3	4:A:605:HOH:O	2.12	0.49
1:C:380:TYR:CE1	1:C:385:ALA:HB2	2.49	0.48
1:D:405:ILE:HD11	1:D:424:LEU:HD11	1.95	0.48
1:F:405:ILE:HD11	1:F:424:LEU:HD11	1.95	0.48
1:C:257:GLY:HA3	3:D:502:EDO:H22	1.95	0.48
1:B:214:PRO:HB2	4:B:643:HOH:O	2.14	0.48
1:C:455:GLU:OE1	1:E:406:SER:OG	2.26	0.48
1:A:141:GLU:O	1:A:145:ARG:HG3	2.13	0.48
1:D:126:MET:O	1:D:150:PHE:HA	2.14	0.47
1:E:380:TYR:CE1	1:E:385:ALA:HB2	2.49	0.47
1:E:68:PHE:HZ	1:E:328:TYR:HD2	1.62	0.47
1:D:151:KCX:OQ1	1:D:184:HIS:HB2	2.15	0.47
1:B:141:GLU:O	1:B:145[A]:ARG:HG2	2.15	0.47
1:C:19:ASP:OD2	4:C:672:HOH:O	2.21	0.47
1:E:61:HIS:CD2	1:E:317:ASP:HA	2.50	0.47
1:B:405:ILE:HD11	1:B:424:LEU:HD11	1.98	0.46
1:C:208:ALA:HA	1:C:211:TYR:CD2	2.51	0.46
1:F:404:LYS:HE3	1:F:421:GLY:HA2	1.97	0.45
1:A:431:THR:HB	1:A:439:PHE:HB3	1.98	0.45
1:D:286:ARG:HG2	1:D:416:TYR:CZ	2.52	0.45
1:A:55:PRO:HG3	1:A:386:VAL:HG23	1.99	0.45
1:C:61:HIS:CD2	1:C:317:ASP:HA	2.52	0.45
1:E:126:MET:O	1:E:150:PHE:HA	2.16	0.45
1:D:61:HIS:CD2	1:D:317:ASP:HA	2.51	0.45
1:C:431:THR:HB	1:C:439:PHE:HB3	1.99	0.44
1:A:61:HIS:CD2	1:A:317:ASP:HA	2.53	0.44
1:A:208:ALA:HA	1:A:211:TYR:CD2	2.53	0.44
1:F:126:MET:O	1:F:150:PHE:HA	2.17	0.43
1:E:55:PRO:HG3	1:E:386:VAL:HG23	2.00	0.43
1:E:145[B]:ARG:NH1	4:E:747:HOH:O	2.43	0.43
1:B:126:MET:O	1:B:150:PHE:HA	2.18	0.43
1:A:126:MET:O	1:A:150:PHE:HA	2.19	0.42
1:A:475:PRO:HB2	1:C:211:TYR:CD2	2.56	0.41
1:E:184:HIS:C	1:E:184:HIS:CD2	2.94	0.41
1:C:126:MET:O	1:C:150:PHE:HA	2.21	0.40
1:A:472:ILE:CD1	1:B:357:THR:HA	2.51	0.40
1:E:353:ARG:HD3	1:E:353:ARG:HA	1.86	0.40
1:A:16:ILE:HB	1:A:54:MET:HG2	2.03	0.40
1:D:208:ALA:HA	1:D:211:TYR:CD2	2.57	0.40
1:F:183:VAL:O	1:F:239:VAL:HG22	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	474/497 (95%)	460 (97%)	14 (3%)	0	100	100
1	B	478/497 (96%)	464 (97%)	14 (3%)	0	100	100
1	C	475/497 (96%)	460 (97%)	15 (3%)	0	100	100
1	D	482/497 (97%)	467 (97%)	15 (3%)	0	100	100
1	E	478/497 (96%)	463 (97%)	15 (3%)	0	100	100
1	F	481/497 (97%)	466 (97%)	15 (3%)	0	100	100
All	All	2868/2982 (96%)	2780 (97%)	88 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/398 (93%)	370 (100%)	0	100	100
1	B	377/398 (95%)	376 (100%)	1 (0%)	92	95
1	C	371/398 (93%)	371 (100%)	0	100	100
1	D	376/398 (94%)	375 (100%)	1 (0%)	92	95
1	E	376/398 (94%)	375 (100%)	1 (0%)	92	95
1	F	368/398 (92%)	368 (100%)	0	100	100
All	All	2238/2388 (94%)	2235 (100%)	3 (0%)	93	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	68	PHE
1	D	68	PHE
1	E	68	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	338	ASN
1	D	277	HIS
1	D	338	ASN
1	E	277	HIS
1	E	338	ASN
1	F	338	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	151	1,2	7,11,12	0.93	0	4,12,14	1.67	1 (25%)
1	KCX	A	151	1,2	7,11,12	1.00	0	4,12,14	1.39	1 (25%)
1	KCX	E	151	1,2	7,11,12	0.97	0	4,12,14	1.50	1 (25%)
1	KCX	D	151	1,2	7,11,12	0.94	0	4,12,14	1.72	1 (25%)
1	KCX	B	151	1,2	7,11,12	1.03	0	4,12,14	1.47	0
1	KCX	F	151	1,2	7,11,12	0.91	0	4,12,14	1.94	1 (25%)

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	151	1,2	-	0/7/10/12	-
1	KCX	A	151	1,2	-	0/7/10/12	-
1	KCX	E	151	1,2	-	0/7/10/12	-
1	KCX	D	151	1,2	-	0/7/10/12	-
1	KCX	B	151	1,2	-	0/7/10/12	-
1	KCX	F	151	1,2	-	0/7/10/12	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	151	KCX	CE-NZ-CX	-3.08	117.74	122.95
1	C	151	KCX	CE-NZ-CX	-2.59	118.56	122.95
1	E	151	KCX	CE-NZ-CX	-2.49	118.72	122.95
1	D	151	KCX	CE-NZ-CX	-2.21	119.20	122.95
1	A	151	KCX	CE-NZ-CX	-2.02	119.52	122.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	151	KCX	1	0
1	D	151	KCX	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 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	EDO	A	506	-	3,3,3	0.44	0	2,2,2	0.30	0
3	EDO	C	505	-	3,3,3	0.48	0	2,2,2	0.36	0
3	EDO	F	503	-	3,3,3	0.43	0	2,2,2	0.68	0
3	EDO	B	502	-	3,3,3	0.46	0	2,2,2	0.22	0
3	EDO	F	505	-	3,3,3	0.41	0	2,2,2	0.36	0
3	EDO	F	504	-	3,3,3	0.50	0	2,2,2	0.54	0
3	EDO	C	504	-	3,3,3	0.40	0	2,2,2	0.89	0
3	EDO	D	503	-	3,3,3	0.51	0	2,2,2	0.57	0
3	EDO	B	503	-	3,3,3	0.49	0	2,2,2	0.51	0
3	EDO	E	505	-	3,3,3	0.54	0	2,2,2	0.27	0
3	EDO	C	502	-	3,3,3	0.56	0	2,2,2	0.08	0
3	EDO	E	503	-	3,3,3	0.43	0	2,2,2	0.68	0
3	EDO	A	503	-	3,3,3	0.44	0	2,2,2	0.36	0
3	EDO	B	504	-	3,3,3	0.33	0	2,2,2	0.96	0
3	EDO	C	503	-	3,3,3	0.46	0	2,2,2	0.57	0
3	EDO	D	504	-	3,3,3	0.39	0	2,2,2	0.58	0
3	EDO	A	505	-	3,3,3	0.44	0	2,2,2	0.53	0
3	EDO	E	502	-	3,3,3	0.46	0	2,2,2	0.30	0
3	EDO	F	502	-	3,3,3	0.46	0	2,2,2	0.24	0
3	EDO	A	507	-	3,3,3	0.49	0	2,2,2	0.34	0
3	EDO	D	505	-	3,3,3	0.39	0	2,2,2	0.39	0
3	EDO	A	504	-	3,3,3	0.47	0	2,2,2	0.64	0
3	EDO	E	504	-	3,3,3	0.35	0	2,2,2	0.95	0
3	EDO	D	502	-	3,3,3	0.49	0	2,2,2	0.28	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
3	EDO	A	506	-	-	0/1/1/1	-
3	EDO	C	505	-	-	0/1/1/1	-
3	EDO	F	503	-	-	1/1/1/1	-
3	EDO	B	502	-	-	0/1/1/1	-
3	EDO	F	505	-	-	0/1/1/1	-
3	EDO	F	504	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	504	-	-	1/1/1/1	-
3	EDO	D	503	-	-	1/1/1/1	-
3	EDO	B	503	-	-	0/1/1/1	-
3	EDO	E	505	-	-	0/1/1/1	-
3	EDO	C	502	-	-	1/1/1/1	-
3	EDO	E	503	-	-	0/1/1/1	-
3	EDO	A	503	-	-	0/1/1/1	-
3	EDO	B	504	-	-	1/1/1/1	-
3	EDO	C	503	-	-	1/1/1/1	-
3	EDO	D	504	-	-	1/1/1/1	-
3	EDO	A	505	-	-	1/1/1/1	-
3	EDO	E	502	-	-	0/1/1/1	-
3	EDO	F	502	-	-	0/1/1/1	-
3	EDO	A	507	-	-	0/1/1/1	-
3	EDO	D	505	-	-	0/1/1/1	-
3	EDO	A	504	-	-	1/1/1/1	-
3	EDO	E	504	-	-	1/1/1/1	-
3	EDO	D	502	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	504	EDO	O1-C1-C2-O2
3	C	503	EDO	O1-C1-C2-O2
3	B	504	EDO	O1-C1-C2-O2
3	F	503	EDO	O1-C1-C2-O2
3	E	504	EDO	O1-C1-C2-O2
3	F	504	EDO	O1-C1-C2-O2
3	A	505	EDO	O1-C1-C2-O2
3	A	504	EDO	O1-C1-C2-O2
3	D	504	EDO	O1-C1-C2-O2
3	D	503	EDO	O1-C1-C2-O2
3	D	502	EDO	O1-C1-C2-O2
3	C	502	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	505	EDO	1	0
3	E	505	EDO	1	0
3	D	502	EDO	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, 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	476/497 (95%)	0.04	23 (4%) 30 39	23, 39, 58, 83	0
1	B	476/497 (95%)	-0.25	9 (1%) 66 74	21, 33, 54, 93	0
1	C	475/497 (95%)	-0.06	11 (2%) 60 68	22, 38, 58, 91	0
1	D	480/497 (96%)	-0.33	8 (1%) 70 76	22, 36, 59, 88	0
1	E	476/497 (95%)	-0.27	6 (1%) 77 82	21, 35, 56, 89	0
1	F	480/497 (96%)	0.01	17 (3%) 44 52	25, 43, 66, 103	0
All	All	2863/2982 (96%)	-0.14	74 (2%) 56 64	21, 37, 59, 103	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	6	ALA	5.0
1	A	482	ALA	4.8
1	F	485	MET	4.7
1	F	484	HIS	4.5
1	A	6	ALA	4.5
1	E	68	PHE	4.5
1	B	482	ALA	4.2
1	F	71	THR	4.0
1	E	328	TYR	3.9
1	C	478	VAL	3.8
1	D	482	ALA	3.7
1	B	68	PHE	3.6
1	A	69	MET	3.6
1	F	486	PRO	3.5
1	D	484	HIS	3.5
1	C	6	ALA	3.3
1	A	281	TRP	3.2
1	B	328	TYR	3.2
1	F	70	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	481	SER	3.2
1	D	486	PRO	3.1
1	A	40	LEU	3.0
1	A	330	ILE	3.0
1	D	328	TYR	2.9
1	F	481	SER	2.9
1	F	478	VAL	2.9
1	A	202	GLY	2.9
1	A	250	ILE	2.8
1	C	68	PHE	2.8
1	A	68	PHE	2.7
1	A	311	LEU	2.7
1	F	482	ALA	2.7
1	D	485	MET	2.7
1	A	306	LEU	2.6
1	F	72	TYR	2.6
1	C	42	GLY	2.5
1	A	376	ILE	2.5
1	A	368	VAL	2.5
1	A	284	ALA	2.4
1	A	279	ARG	2.4
1	A	308	ALA	2.4
1	C	71	THR	2.4
1	E	481	SER	2.4
1	D	70	GLY	2.4
1	C	329	GLY	2.4
1	A	45	VAL	2.4
1	F	477	LYS	2.4
1	A	481	SER	2.3
1	B	307	ALA	2.3
1	A	307	ALA	2.3
1	F	330	ILE	2.3
1	A	310	SER	2.3
1	E	45	VAL	2.2
1	B	40	LEU	2.2
1	E	309	GLY	2.2
1	B	306	LEU	2.1
1	A	200	ALA	2.1
1	D	481	SER	2.1
1	D	71	THR	2.1
1	C	330	ILE	2.1
1	F	68	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	69	MET	2.1
1	B	250	ILE	2.1
1	B	309	GLY	2.1
1	A	336	ILE	2.1
1	C	278	ASN	2.1
1	C	480	ARG	2.1
1	A	283	TYR	2.1
1	C	306	LEU	2.0
1	F	250	ILE	2.0
1	F	45	VAL	2.0
1	F	328	TYR	2.0
1	E	6	ALA	2.0
1	B	311	LEU	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, 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
1	KCX	F	151	12/13	0.94	0.09	31,35,45,54	0
1	KCX	B	151	12/13	0.96	0.08	25,29,36,42	0
1	KCX	E	151	12/13	0.96	0.07	22,28,33,38	0
1	KCX	C	151	12/13	0.97	0.09	29,33,43,48	0
1	KCX	D	151	12/13	0.97	0.08	24,28,40,44	0
1	KCX	A	151	12/13	0.98	0.09	27,33,36,42	0

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(\AA^2)	Q<0.9
3	EDO	E	505	4/4	0.87	0.18	36,38,41,50	0
3	EDO	B	503	4/4	0.89	0.33	38,39,45,47	0
3	EDO	C	505	4/4	0.89	0.19	35,43,45,58	0
3	EDO	F	502	4/4	0.90	0.16	43,49,49,49	0
3	EDO	A	507	4/4	0.90	0.21	39,46,49,51	0
3	EDO	A	506	4/4	0.92	0.22	32,34,40,53	0
3	EDO	F	505	4/4	0.93	0.17	40,45,45,55	0
3	EDO	D	503	4/4	0.94	0.20	42,43,44,45	0
3	EDO	F	504	4/4	0.94	0.15	43,49,51,52	0
3	EDO	C	503	4/4	0.94	0.24	35,41,41,41	0
3	EDO	D	505	4/4	0.94	0.24	44,45,46,53	0
3	EDO	E	502	4/4	0.95	0.15	44,50,50,53	0
3	EDO	E	503	4/4	0.95	0.22	40,41,46,46	0
3	EDO	A	504	4/4	0.95	0.33	36,40,41,43	0
3	EDO	D	502	4/4	0.95	0.17	40,46,49,51	0
3	EDO	C	502	4/4	0.96	0.18	36,44,44,45	0
3	EDO	C	504	4/4	0.96	0.23	44,47,47,47	0
3	EDO	A	503	4/4	0.96	0.18	37,44,50,50	0
3	EDO	B	504	4/4	0.96	0.15	39,41,43,46	0
3	EDO	F	503	4/4	0.97	0.19	36,41,41,44	0
2	ZN	D	500	1/1	0.97	0.06	46,46,46,46	0
3	EDO	B	502	4/4	0.97	0.16	32,42,47,48	0
2	ZN	F	500	1/1	0.98	0.04	53,53,53,53	0
3	EDO	A	505	4/4	0.98	0.18	37,37,39,43	0
2	ZN	C	501	1/1	0.98	0.06	53,53,53,53	0
2	ZN	A	502	1/1	0.99	0.07	50,50,50,50	0
2	ZN	C	500	1/1	0.99	0.07	51,51,51,51	0
2	ZN	E	501	1/1	0.99	0.05	51,51,51,51	0
2	ZN	F	501	1/1	0.99	0.04	56,56,56,56	0
2	ZN	A	501	1/1	0.99	0.06	47,47,47,47	0
3	EDO	E	504	4/4	0.99	0.16	42,43,45,51	0
2	ZN	D	501	1/1	0.99	0.04	50,50,50,50	0
2	ZN	E	500	1/1	0.99	0.06	45,45,45,45	0
2	ZN	B	501	1/1	0.99	0.06	48,48,48,48	0
3	EDO	D	504	4/4	0.99	0.13	39,40,44,50	0
2	ZN	B	500	1/1	1.00	0.06	44,44,44,44	0

6.5 Other polymers ⓘ

There are no such residues in this entry.