



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 05:48 AM EDT

PDB ID : 7O0A / pdb_00007o0a
Title : Bdellovibrio bacteriovorus PGI in P1211 spacegroup
Authors : Meek, R.W.; Lovering, A.L.
Deposited on : 2021-03-26
Resolution : 1.74 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

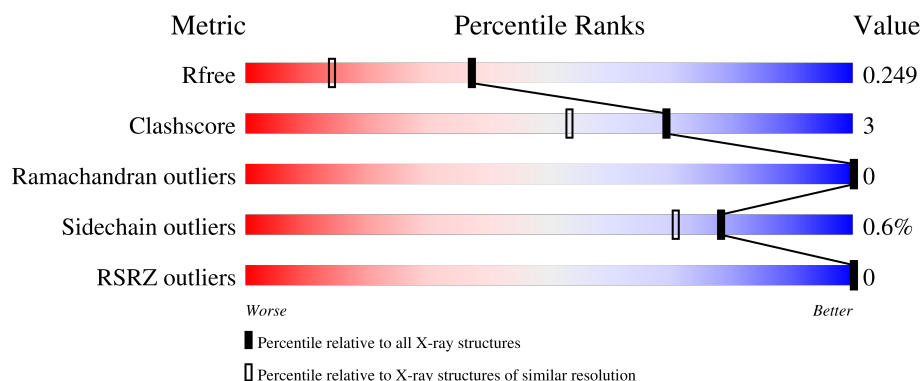
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

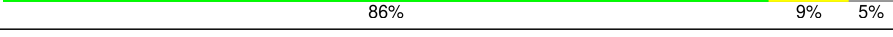
The reported resolution of this entry is 1.74 Å.

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}	180053	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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 $\leq 5\%$. 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	428	 88% 6% 6%
1	B	428	 86% 9% 5%
1	C	428	 88% 6% 6%
1	D	428	 86% 9% 5%
1	E	428	 88% 6% 5%

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Mol	Chain	Length	Quality of chain
1	F	428	
1	G	428	
1	H	428	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	E	601	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29338 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 Glucose-6-phosphate isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	6	0
			3222	2057	539	607	19			
1	B	405	Total	C	N	O	S	0	11	0
			3278	2093	549	614	22			
1	C	404	Total	C	N	O	S	0	12	0
			3263	2083	545	616	19			
1	D	405	Total	C	N	O	S	0	12	0
			3287	2103	550	612	22			
1	F	405	Total	C	N	O	S	0	5	0
			3233	2064	546	604	19			
1	G	404	Total	C	N	O	S	0	9	0
			3245	2071	547	608	19			
1	H	404	Total	C	N	O	S	0	8	0
			3242	2070	545	605	22			
1	E	405	Total	C	N	O	S	0	13	0
			3290	2100	555	614	21			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	409	LEU	-	expression tag	UNP Q6MPU9
A	410	VAL	-	expression tag	UNP Q6MPU9
A	411	PRO	-	expression tag	UNP Q6MPU9
A	412	ARG	-	expression tag	UNP Q6MPU9
A	413	GLY	-	expression tag	UNP Q6MPU9
A	414	SER	-	expression tag	UNP Q6MPU9
A	415	ALA	-	expression tag	UNP Q6MPU9
A	416	ALA	-	expression tag	UNP Q6MPU9
A	417	ALA	-	expression tag	UNP Q6MPU9
A	418	ALA	-	expression tag	UNP Q6MPU9
A	419	LEU	-	expression tag	UNP Q6MPU9
A	420	GLU	-	expression tag	UNP Q6MPU9
A	421	HIS	-	expression tag	UNP Q6MPU9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	422	HIS	-	expression tag	UNP Q6MPU9
A	423	HIS	-	expression tag	UNP Q6MPU9
A	424	HIS	-	expression tag	UNP Q6MPU9
A	425	HIS	-	expression tag	UNP Q6MPU9
A	426	HIS	-	expression tag	UNP Q6MPU9
A	427	HIS	-	expression tag	UNP Q6MPU9
A	428	HIS	-	expression tag	UNP Q6MPU9
B	409	LEU	-	expression tag	UNP Q6MPU9
B	410	VAL	-	expression tag	UNP Q6MPU9
B	411	PRO	-	expression tag	UNP Q6MPU9
B	412	ARG	-	expression tag	UNP Q6MPU9
B	413	GLY	-	expression tag	UNP Q6MPU9
B	414	SER	-	expression tag	UNP Q6MPU9
B	415	ALA	-	expression tag	UNP Q6MPU9
B	416	ALA	-	expression tag	UNP Q6MPU9
B	417	ALA	-	expression tag	UNP Q6MPU9
B	418	ALA	-	expression tag	UNP Q6MPU9
B	419	LEU	-	expression tag	UNP Q6MPU9
B	420	GLU	-	expression tag	UNP Q6MPU9
B	421	HIS	-	expression tag	UNP Q6MPU9
B	422	HIS	-	expression tag	UNP Q6MPU9
B	423	HIS	-	expression tag	UNP Q6MPU9
B	424	HIS	-	expression tag	UNP Q6MPU9
B	425	HIS	-	expression tag	UNP Q6MPU9
B	426	HIS	-	expression tag	UNP Q6MPU9
B	427	HIS	-	expression tag	UNP Q6MPU9
B	428	HIS	-	expression tag	UNP Q6MPU9
C	409	LEU	-	expression tag	UNP Q6MPU9
C	410	VAL	-	expression tag	UNP Q6MPU9
C	411	PRO	-	expression tag	UNP Q6MPU9
C	412	ARG	-	expression tag	UNP Q6MPU9
C	413	GLY	-	expression tag	UNP Q6MPU9
C	414	SER	-	expression tag	UNP Q6MPU9
C	415	ALA	-	expression tag	UNP Q6MPU9
C	416	ALA	-	expression tag	UNP Q6MPU9
C	417	ALA	-	expression tag	UNP Q6MPU9
C	418	ALA	-	expression tag	UNP Q6MPU9
C	419	LEU	-	expression tag	UNP Q6MPU9
C	420	GLU	-	expression tag	UNP Q6MPU9
C	421	HIS	-	expression tag	UNP Q6MPU9
C	422	HIS	-	expression tag	UNP Q6MPU9
C	423	HIS	-	expression tag	UNP Q6MPU9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	424	HIS	-	expression tag	UNP Q6MPU9
C	425	HIS	-	expression tag	UNP Q6MPU9
C	426	HIS	-	expression tag	UNP Q6MPU9
C	427	HIS	-	expression tag	UNP Q6MPU9
C	428	HIS	-	expression tag	UNP Q6MPU9
D	409	LEU	-	expression tag	UNP Q6MPU9
D	410	VAL	-	expression tag	UNP Q6MPU9
D	411	PRO	-	expression tag	UNP Q6MPU9
D	412	ARG	-	expression tag	UNP Q6MPU9
D	413	GLY	-	expression tag	UNP Q6MPU9
D	414	SER	-	expression tag	UNP Q6MPU9
D	415	ALA	-	expression tag	UNP Q6MPU9
D	416	ALA	-	expression tag	UNP Q6MPU9
D	417	ALA	-	expression tag	UNP Q6MPU9
D	418	ALA	-	expression tag	UNP Q6MPU9
D	419	LEU	-	expression tag	UNP Q6MPU9
D	420	GLU	-	expression tag	UNP Q6MPU9
D	421	HIS	-	expression tag	UNP Q6MPU9
D	422	HIS	-	expression tag	UNP Q6MPU9
D	423	HIS	-	expression tag	UNP Q6MPU9
D	424	HIS	-	expression tag	UNP Q6MPU9
D	425	HIS	-	expression tag	UNP Q6MPU9
D	426	HIS	-	expression tag	UNP Q6MPU9
D	427	HIS	-	expression tag	UNP Q6MPU9
D	428	HIS	-	expression tag	UNP Q6MPU9
F	409	LEU	-	expression tag	UNP Q6MPU9
F	410	VAL	-	expression tag	UNP Q6MPU9
F	411	PRO	-	expression tag	UNP Q6MPU9
F	412	ARG	-	expression tag	UNP Q6MPU9
F	413	GLY	-	expression tag	UNP Q6MPU9
F	414	SER	-	expression tag	UNP Q6MPU9
F	415	ALA	-	expression tag	UNP Q6MPU9
F	416	ALA	-	expression tag	UNP Q6MPU9
F	417	ALA	-	expression tag	UNP Q6MPU9
F	418	ALA	-	expression tag	UNP Q6MPU9
F	419	LEU	-	expression tag	UNP Q6MPU9
F	420	GLU	-	expression tag	UNP Q6MPU9
F	421	HIS	-	expression tag	UNP Q6MPU9
F	422	HIS	-	expression tag	UNP Q6MPU9
F	423	HIS	-	expression tag	UNP Q6MPU9
F	424	HIS	-	expression tag	UNP Q6MPU9
F	425	HIS	-	expression tag	UNP Q6MPU9

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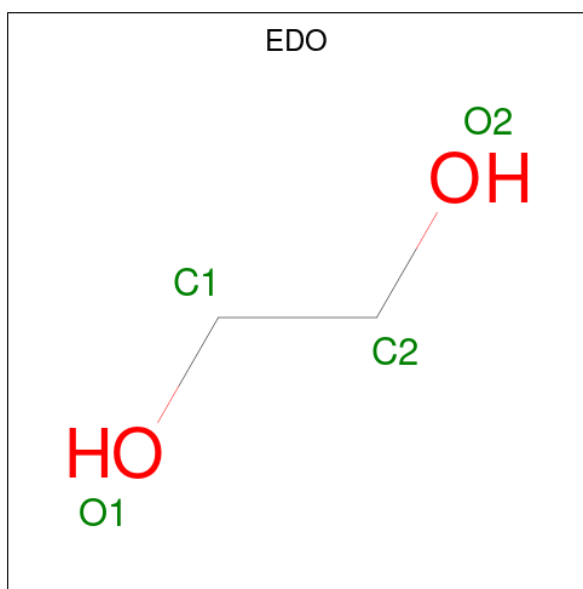
Chain	Residue	Modelled	Actual	Comment	Reference
F	426	HIS	-	expression tag	UNP Q6MPU9
F	427	HIS	-	expression tag	UNP Q6MPU9
F	428	HIS	-	expression tag	UNP Q6MPU9
G	409	LEU	-	expression tag	UNP Q6MPU9
G	410	VAL	-	expression tag	UNP Q6MPU9
G	411	PRO	-	expression tag	UNP Q6MPU9
G	412	ARG	-	expression tag	UNP Q6MPU9
G	413	GLY	-	expression tag	UNP Q6MPU9
G	414	SER	-	expression tag	UNP Q6MPU9
G	415	ALA	-	expression tag	UNP Q6MPU9
G	416	ALA	-	expression tag	UNP Q6MPU9
G	417	ALA	-	expression tag	UNP Q6MPU9
G	418	ALA	-	expression tag	UNP Q6MPU9
G	419	LEU	-	expression tag	UNP Q6MPU9
G	420	GLU	-	expression tag	UNP Q6MPU9
G	421	HIS	-	expression tag	UNP Q6MPU9
G	422	HIS	-	expression tag	UNP Q6MPU9
G	423	HIS	-	expression tag	UNP Q6MPU9
G	424	HIS	-	expression tag	UNP Q6MPU9
G	425	HIS	-	expression tag	UNP Q6MPU9
G	426	HIS	-	expression tag	UNP Q6MPU9
G	427	HIS	-	expression tag	UNP Q6MPU9
G	428	HIS	-	expression tag	UNP Q6MPU9
H	409	LEU	-	expression tag	UNP Q6MPU9
H	410	VAL	-	expression tag	UNP Q6MPU9
H	411	PRO	-	expression tag	UNP Q6MPU9
H	412	ARG	-	expression tag	UNP Q6MPU9
H	413	GLY	-	expression tag	UNP Q6MPU9
H	414	SER	-	expression tag	UNP Q6MPU9
H	415	ALA	-	expression tag	UNP Q6MPU9
H	416	ALA	-	expression tag	UNP Q6MPU9
H	417	ALA	-	expression tag	UNP Q6MPU9
H	418	ALA	-	expression tag	UNP Q6MPU9
H	419	LEU	-	expression tag	UNP Q6MPU9
H	420	GLU	-	expression tag	UNP Q6MPU9
H	421	HIS	-	expression tag	UNP Q6MPU9
H	422	HIS	-	expression tag	UNP Q6MPU9
H	423	HIS	-	expression tag	UNP Q6MPU9
H	424	HIS	-	expression tag	UNP Q6MPU9
H	425	HIS	-	expression tag	UNP Q6MPU9
H	426	HIS	-	expression tag	UNP Q6MPU9
H	427	HIS	-	expression tag	UNP Q6MPU9

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Chain	Residue	Modelled	Actual	Comment	Reference
H	428	HIS	-	expression tag	UNP Q6MPU9
E	409	LEU	-	expression tag	UNP Q6MPU9
E	410	VAL	-	expression tag	UNP Q6MPU9
E	411	PRO	-	expression tag	UNP Q6MPU9
E	412	ARG	-	expression tag	UNP Q6MPU9
E	413	GLY	-	expression tag	UNP Q6MPU9
E	414	SER	-	expression tag	UNP Q6MPU9
E	415	ALA	-	expression tag	UNP Q6MPU9
E	416	ALA	-	expression tag	UNP Q6MPU9
E	417	ALA	-	expression tag	UNP Q6MPU9
E	418	ALA	-	expression tag	UNP Q6MPU9
E	419	LEU	-	expression tag	UNP Q6MPU9
E	420	GLU	-	expression tag	UNP Q6MPU9
E	421	HIS	-	expression tag	UNP Q6MPU9
E	422	HIS	-	expression tag	UNP Q6MPU9
E	423	HIS	-	expression tag	UNP Q6MPU9
E	424	HIS	-	expression tag	UNP Q6MPU9
E	425	HIS	-	expression tag	UNP Q6MPU9
E	426	HIS	-	expression tag	UNP Q6MPU9
E	427	HIS	-	expression tag	UNP Q6MPU9
E	428	HIS	-	expression tag	UNP Q6MPU9

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



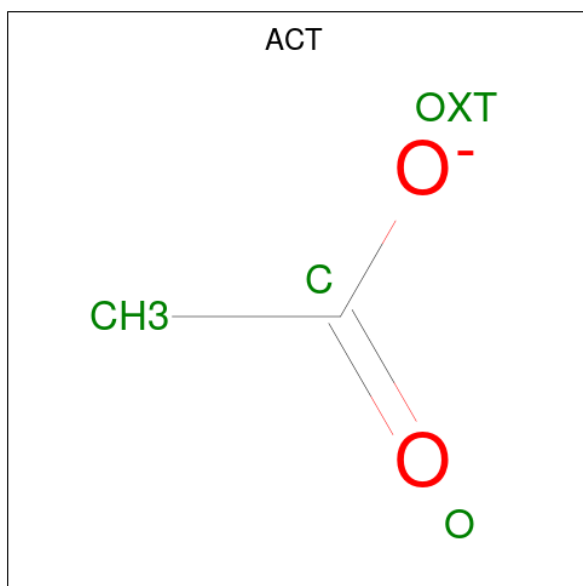
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	399	Total	O	0	0
			399	399		
4	B	410	Total	O	0	0
			410	410		
4	C	412	Total	O	0	0
			412	412		
4	D	463	Total	O	0	0
			463	463		

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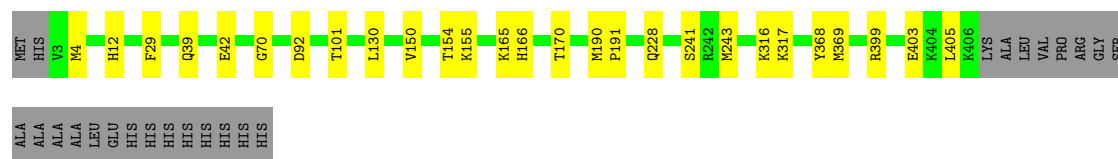
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	449	Total 449	O 449	0	0
4	G	408	Total 408	O 408	0	0
4	H	340	Total 340	O 340	0	0
4	E	373	Total 373	O 373	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

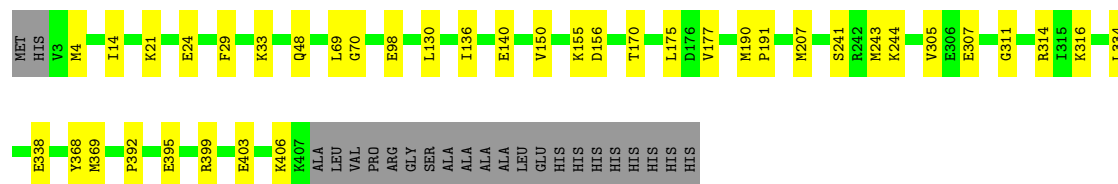
- Molecule 1: Glucose-6-phosphate isomerase

Chain A: 



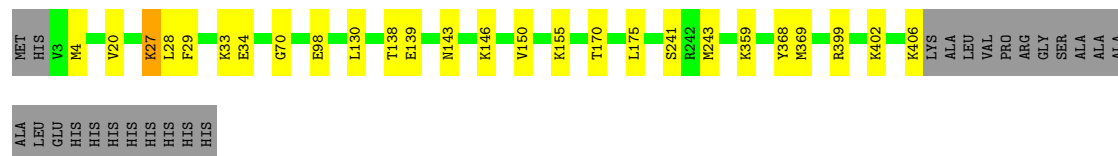
- Molecule 1: Glucose-6-phosphate isomerase

Chain B: 



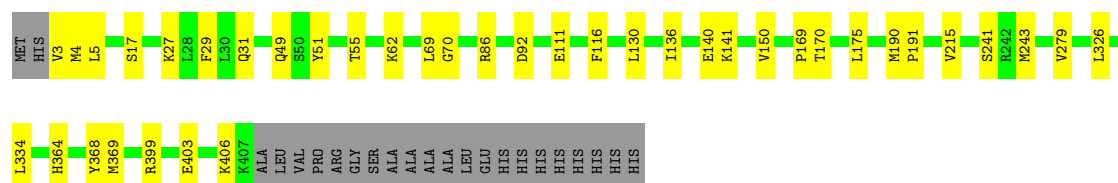
- Molecule 1: Glucose-6-phosphate isomerase

Chain C: 



- Molecule 1: Glucose-6-phosphate isomerase

Chain D: 



- [illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	137.92Å 118.10Å 138.98Å 90.00° 118.41° 90.00°	Depositor
Resolution (Å)	59.54 – 1.74 59.54 – 1.74	Depositor EDS
% Data completeness (in resolution range)	98.7 (59.54-1.74) 85.1 (59.54-1.74)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.222 , 0.253 0.220 , 0.249	Depositor DCC
R_{free} test set	20056 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 25.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.064 for -h-l,k,h 0.064 for l,k,-h-l 0.146 for h,-k,-h-l 0.066 for -h-l,-k,l 0.068 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	29338	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.26% 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: EDO, ACT

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	0.98	0/3289	1.26	4/4434 (0.1%)
1	B	0.98	0/3342	1.26	4/4502 (0.1%)
1	C	0.96	0/3333	1.23	1/4494 (0.0%)
1	D	0.99	0/3354	1.25	1/4515 (0.0%)
1	E	0.97	0/3354	1.24	3/4516 (0.1%)
1	F	0.98	0/3294	1.25	3/4438 (0.1%)
1	G	0.97	0/3312	1.24	2/4462 (0.0%)
1	H	0.96	0/3306	1.25	3/4453 (0.1%)
All	All	0.97	0/26584	1.25	21/35814 (0.1%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	405	LEU	CA-C-N	6.80	133.93	121.70
1	A	405	LEU	C-N-CA	6.80	133.93	121.70
1	A	405	LEU	O-C-N	6.46	130.29	122.35
1	F	311	GLY	CA-C-O	-6.31	118.12	122.22
1	C	29	PHE	CA-CB-CG	-6.13	107.67	113.80
1	F	29	PHE	CA-CB-CG	-6.12	107.68	113.80
1	H	29	PHE	CA-CB-CG	-6.11	107.69	113.80
1	A	29	PHE	CA-CB-CG	-6.07	107.73	113.80
1	B	29	PHE	CA-CB-CG	-5.93	107.87	113.80
1	G	29	PHE	CA-CB-CG	-5.89	107.91	113.80
1	B	177	VAL	CA-C-N	5.86	125.91	120.34
1	B	177	VAL	C-N-CA	5.86	125.91	120.34
1	D	29	PHE	CA-CB-CG	-5.71	108.09	113.80
1	E	29	PHE	CA-CB-CG	-5.57	108.23	113.80
1	B	311	GLY	CA-C-O	-5.55	118.61	122.22
1	G	311	GLY	CA-C-O	-5.54	118.62	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	311	GLY	CA-C-O	-5.48	118.66	122.22
1	F	395	GLU	CB-CG-CD	5.19	121.43	112.60
1	H	307	GLU	N-CA-CB	-5.17	102.52	110.12
1	E	178	GLY	CA-C-N	5.03	125.67	119.99
1	E	178	GLY	C-N-CA	5.03	125.67	119.99

There are no chirality outliers.

There are no planarity outliers.

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	3222	0	3264	22	0
1	B	3278	0	3328	34	0
1	C	3263	0	3304	24	0
1	D	3287	0	3352	42	0
1	E	3290	0	3349	19	0
1	F	3233	0	3285	24	0
1	G	3245	0	3298	20	0
1	H	3242	0	3293	23	0
2	C	4	0	6	0	0
2	D	4	0	6	0	0
3	D	8	0	6	1	0
3	E	4	0	3	3	0
3	F	4	0	3	0	0
4	A	399	0	0	5	0
4	B	410	0	0	8	0
4	C	412	0	0	7	0
4	D	463	0	0	10	0
4	E	373	0	0	5	0
4	F	449	0	0	5	0
4	G	408	0	0	6	0
4	H	340	0	0	5	0
All	All	29338	0	26497	183	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 3.

All (183) 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:3:VAL:C	1:D:4[C]:MET:CA	2.49	0.84
1:C:34:GLU:OE1	1:D:17:SER:HB3	1.81	0.80
1:E:219[B]:THR:HG21	1:E:372:PHE:HZ	1.46	0.79
1:B:244[B]:LYS:HE2	4:B:578:HOH:O	1.81	0.78
1:D:4[C]:MET:CA	1:D:5:LEU:N	2.46	0.78
1:H:74:LEU:HD12	1:H:249:TRP:HB2	1.66	0.78
1:D:62[B]:LYS:HD2	1:D:111:GLU:OE1	1.84	0.77
1:E:215:VAL:O	1:E:219[B]:THR:HG23	1.85	0.76
1:D:55[B]:THR:HG22	4:D:820:HOH:O	1.87	0.74
1:D:70:GLY:HA2	4:D:836:HOH:O	1.90	0.71
1:C:70:GLY:HA2	4:C:824:HOH:O	1.94	0.68
1:G:70:GLY:HA2	4:G:523:HOH:O	1.93	0.67
1:C:34:GLU:OE1	1:D:17:SER:CB	2.43	0.67
1:D:116:PHE:CZ	1:D:130[B]:LEU:HD23	2.30	0.67
1:H:74:LEU:O	1:H:74:LEU:HD13	1.95	0.66
4:C:932:HOH:O	1:D:31:GLN:HG3	1.95	0.66
1:D:51:TYR:O	1:D:55[B]:THR:HG23	1.99	0.63
1:H:4[B]:MET:HE2	1:H:208[B]:ARG:HE	1.64	0.63
1:C:138:THR:HG21	4:C:850:HOH:O	1.97	0.63
1:D:27:LYS:HD2	4:D:1017:HOH:O	1.99	0.62
1:B:243:MET:CE	1:B:369[A]:MET:HE1	2.30	0.61
1:H:74:LEU:CD1	1:H:249:TRP:HB2	2.28	0.61
1:E:219[B]:THR:HG21	1:E:372:PHE:CZ	2.33	0.61
1:F:51:TYR:O	1:F:55[A]:THR:HG23	2.01	0.60
1:C:243:MET:CE	1:C:369:MET:HE1	2.30	0.60
1:H:243:MET:CE	1:H:369[A]:MET:HE1	2.32	0.60
1:G:243:MET:CE	1:G:369:MET:HE1	2.32	0.60
1:D:243:MET:CE	1:D:369[A]:MET:HE1	2.32	0.60
1:B:70:GLY:HA2	4:B:651:HOH:O	2.02	0.59
1:D:175:LEU:HD21	4:D:911:HOH:O	2.02	0.58
1:B:175:LEU:CD1	1:C:20:VAL:HG21	2.34	0.58
1:F:268:PRO:HG3	1:G:316:LYS:HB3	1.85	0.58
1:H:74:LEU:HD13	1:H:74:LEU:C	2.29	0.58
1:A:243:MET:CE	1:A:369:MET:HE1	2.35	0.57
1:D:403:GLU:HA	1:D:406:LYS:HD2	1.87	0.57
1:D:279:VAL:HG22	4:D:921:HOH:O	2.04	0.57
1:H:74:LEU:HD12	1:H:249:TRP:CB	2.34	0.56
1:C:243:MET:HE1	1:C:369:MET:HE1	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143[B]:ASN:HD22	1:C:146:LYS:HG2	1.69	0.56
1:C:143[B]:ASN:ND2	1:C:146:LYS:HG2	2.20	0.56
1:D:62[A]:LYS:HG3	4:D:896:HOH:O	2.06	0.56
1:D:116:PHE:CE1	1:D:130[B]:LEU:HD23	2.41	0.55
1:B:14:ILE:HG12	4:B:516:HOH:O	2.05	0.55
1:B:243:MET:HE1	1:B:369[A]:MET:HE1	1.88	0.55
1:E:4[B]:MET:HE2	1:E:208:ARG:HD2	1.87	0.55
1:D:4[C]:MET:HG2	1:D:368:TYR:CG	2.42	0.55
1:A:154[A]:THR:HG23	1:B:24[A]:GLU:OE1	2.06	0.55
1:D:334[B]:LEU:HD23	1:F:405:LEU:CD1	2.37	0.55
1:F:4:MET:HG2	1:F:368:TYR:CG	2.42	0.54
1:G:232:TRP:C	1:G:273[B]:SER:OG	2.50	0.54
1:H:165:LYS:HG3	4:H:531:HOH:O	2.06	0.54
1:H:243:MET:HE1	1:H:369[A]:MET:HE1	1.89	0.54
1:E:70:GLY:HA2	4:E:779:HOH:O	2.06	0.54
1:A:70:GLY:HA2	4:A:604:HOH:O	2.06	0.54
1:F:296:LYS:HE3	1:F:349:SER:O	2.06	0.54
1:D:243:MET:HE1	1:D:369[A]:MET:HE1	1.89	0.54
1:B:334:LEU:HD21	4:G:895:HOH:O	2.06	0.53
1:A:4:MET:HG2	1:A:368:TYR:CG	2.44	0.53
1:B:4:MET:HG2	1:B:368:TYR:CG	2.43	0.53
1:D:4[A]:MET:HG2	1:D:368:TYR:CG	2.44	0.52
1:A:243:MET:HE1	1:A:369:MET:HE1	1.91	0.52
1:B:175:LEU:HD12	1:C:20:VAL:HG21	1.92	0.52
1:D:141[B]:LYS:HE3	4:D:963:HOH:O	2.10	0.52
1:G:319:GLN:NE2	4:G:506:HOH:O	2.31	0.52
1:D:4[B]:MET:HG2	1:D:368:TYR:CG	2.44	0.52
1:A:154[A]:THR:HG21	1:B:21:LYS:NZ	2.25	0.51
1:A:228:GLN:HG2	4:A:835:HOH:O	2.11	0.51
1:H:4[A]:MET:HG2	1:H:368:TYR:CG	2.45	0.51
1:C:4:MET:HG2	1:C:368:TYR:CG	2.45	0.51
1:D:326:LEU:HD22	1:D:334[A]:LEU:HD21	1.91	0.51
1:A:241[B]:SER:OG	1:E:98:GLU:OE1	2.29	0.51
1:B:241[B]:SER:OG	1:G:98:GLU:HB2	2.11	0.51
1:G:243:MET:HE1	1:G:369:MET:HE1	1.92	0.50
1:E:99:PHE:HB2	3:E:601:ACT:H1	1.91	0.50
1:B:392:PRO:O	1:B:395:GLU:HG2	2.13	0.49
1:B:399[B]:ARG:NH2	1:B:403:GLU:OE2	2.45	0.49
1:B:156:ASP:OD1	4:B:501:HOH:O	2.20	0.49
1:E:261:PRO:HD2	4:E:977:HOH:O	2.13	0.49
1:A:92:ASP:HB3	4:A:686:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:GLU:OE1	1:H:241[B]:SER:OG	2.30	0.49
1:G:399[B]:ARG:NH2	1:G:403:GLU:OE2	2.46	0.48
1:D:62[B]:LYS:HG2	1:D:111:GLU:HB3	1.96	0.48
1:B:369[A]:MET:HE3	4:B:597:HOH:O	2.14	0.48
1:C:241[B]:SER:OG	1:H:98:GLU:OE1	2.32	0.48
1:G:66:ILE:HB	1:G:90:PHE:CD1	2.49	0.48
1:D:399:ARG:NH1	1:D:403:GLU:OE2	2.47	0.48
1:D:86:ARG:NH2	1:F:105:GLU:OE2	2.32	0.47
1:B:98:GLU:OE1	1:G:241[B]:SER:OG	2.30	0.47
1:D:4[C]:MET:HE1	1:D:364:HIS:HB3	1.96	0.47
1:B:395:GLU:HG2	4:B:702:HOH:O	2.14	0.47
1:D:130[B]:LEU:HD12	1:F:320:PHE:CE2	2.49	0.47
1:A:155:LYS:CA	1:B:24[A]:GLU:OE2	2.62	0.47
1:F:4:MET:CE	1:F:208[A]:ARG:NH2	2.77	0.47
1:E:369[B]:MET:HE3	4:E:768:HOH:O	2.14	0.47
1:C:155:LYS:HB3	4:C:722:HOH:O	2.15	0.47
1:C:27[A]:LYS:N	1:C:27[A]:LYS:HD3	2.29	0.47
1:C:139[B]:GLU:O	1:C:139[B]:GLU:HG2	2.13	0.47
1:G:307:GLU:OE1	4:G:502:HOH:O	2.20	0.47
1:H:225[B]:GLN:NE2	4:H:517:HOH:O	2.43	0.47
1:H:399:ARG:NH1	1:H:403:GLU:OE2	2.47	0.47
1:F:307:GLU:HG3	4:F:632:HOH:O	2.13	0.46
1:A:155:LYS:N	1:B:24[A]:GLU:OE2	2.48	0.46
1:B:155:LYS:HD2	4:C:988:HOH:O	2.15	0.46
1:A:39:GLN:O	1:A:42[A]:GLU:HG2	2.16	0.46
1:A:399:ARG:NH1	1:A:403:GLU:OE2	2.48	0.45
1:B:33:LYS:HA	1:B:33:LYS:HE2	1.97	0.45
1:C:130[A]:LEU:C	1:C:130[A]:LEU:HD23	2.41	0.45
1:D:150:VAL:O	1:D:170:THR:HA	2.16	0.45
1:H:150:VAL:O	1:H:170:THR:HA	2.16	0.45
1:E:150:VAL:O	1:E:170:THR:HA	2.17	0.45
1:F:150:VAL:O	1:F:170:THR:HA	2.17	0.45
1:G:130:LEU:HD23	1:G:130:LEU:C	2.43	0.44
1:G:150:VAL:O	1:G:170:THR:HA	2.16	0.44
1:B:334:LEU:HD22	1:B:338:GLU:OE2	2.18	0.44
1:A:154[A]:THR:HG23	1:B:24[A]:GLU:CD	2.43	0.44
1:C:175:LEU:HD21	4:C:722:HOH:O	2.18	0.44
1:F:130:LEU:C	1:F:130:LEU:HD23	2.43	0.44
1:G:395:GLU:OE1	4:G:501:HOH:O	2.20	0.44
1:B:175:LEU:C	1:B:175:LEU:HD23	2.43	0.44
1:B:314:ARG:NH1	4:B:503:HOH:O	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:VAL:O	1:C:170:THR:HA	2.17	0.44
1:B:98:GLU:CD	1:G:241[B]:SER:HG	2.24	0.44
1:F:51:TYR:CZ	1:F:55[A]:THR:HG21	2.53	0.44
1:B:150:VAL:O	1:B:170:THR:HA	2.17	0.43
1:C:399:ARG:HA	1:C:402:LYS:HE2	2.00	0.43
1:H:130:LEU:C	1:H:130:LEU:HD23	2.43	0.43
1:E:99:PHE:HB2	3:E:601:ACT:CH3	2.48	0.43
1:A:130:LEU:C	1:A:130:LEU:HD23	2.43	0.43
1:B:130:LEU:C	1:B:130:LEU:HD23	2.43	0.43
1:G:49:GLN:NE2	4:G:503:HOH:O	2.24	0.43
1:E:91:VAL:HG13	3:E:601:ACT:H2	2.01	0.43
1:H:4[B]:MET:HE2	1:H:4[B]:MET:HB2	1.92	0.43
1:A:150:VAL:O	1:A:170:THR:HA	2.17	0.43
1:F:70:GLY:HA2	4:F:637:HOH:O	2.18	0.43
1:G:4:MET:HG2	1:G:208[A]:ARG:CZ	2.48	0.43
1:E:130:LEU:C	1:E:130:LEU:HD23	2.44	0.43
1:A:190:MET:HB3	1:A:191:PRO:HD3	2.01	0.43
1:A:316:LYS:HE3	1:E:139:GLU:OE2	2.18	0.43
1:D:190:MET:HB3	1:D:191:PRO:HD3	2.00	0.43
1:H:136:ILE:O	1:H:140:GLU:HG3	2.19	0.43
1:H:74:LEU:CD1	1:H:74:LEU:C	2.92	0.42
1:B:136:ILE:O	1:B:140:GLU:HG3	2.19	0.42
1:F:190:MET:HB3	1:F:191:PRO:HD3	2.00	0.42
1:D:69:LEU:CD2	4:D:785:HOH:O	2.67	0.42
1:E:190:MET:HB3	1:E:191:PRO:HD3	2.02	0.42
1:B:316:LYS:NZ	1:G:139:GLU:OE2	2.41	0.42
1:H:33:LYS:HD2	4:H:783:HOH:O	2.20	0.42
1:D:215:VAL:HG23	3:D:502:ACT:H2	2.02	0.42
1:B:305:VAL:HG12	1:B:307[B]:GLU:HG2	2.01	0.42
1:G:190:MET:HB3	1:G:191:PRO:HD3	2.02	0.42
1:H:175:LEU:HD13	4:H:720:HOH:O	2.19	0.42
1:H:190:MET:HB3	1:H:191:PRO:HD3	2.02	0.42
1:B:69:LEU:CD2	4:B:633:HOH:O	2.67	0.42
1:A:12:HIS:CE1	4:A:731:HOH:O	2.73	0.42
1:C:359:LYS:HG2	4:C:795:HOH:O	2.18	0.42
1:F:28:LEU:O	1:F:28:LEU:HD23	2.20	0.42
1:F:136:ILE:O	1:F:140:GLU:HG3	2.20	0.42
1:E:402:LYS:NZ	4:E:743:HOH:O	2.53	0.41
1:D:51:TYR:CZ	1:D:55[B]:THR:HG21	2.55	0.41
1:D:169:PRO:HG3	4:D:973:HOH:O	2.18	0.41
1:C:27[A]:LYS:HD2	1:C:27[A]:LYS:HA	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:ILE:O	1:D:140:GLU:HG3	2.20	0.41
1:D:241[B]:SER:OG	1:F:98:GLU:CD	2.63	0.41
1:F:3:VAL:O	1:F:3:VAL:HG13	2.19	0.41
1:A:165:LYS:HD3	1:A:166:HIS:CE1	2.55	0.41
1:C:143[B]:ASN:HD22	1:C:146:LYS:CG	2.33	0.41
1:F:268:PRO:CG	1:G:316:LYS:HB3	2.50	0.41
1:A:369:MET:HE3	4:A:627:HOH:O	2.21	0.41
1:D:92:ASP:HB3	4:D:804:HOH:O	2.21	0.41
1:F:395:GLU:HG2	4:F:855:HOH:O	2.20	0.41
1:C:130[A]:LEU:HD23	1:C:130[A]:LEU:O	2.21	0.41
1:D:334[B]:LEU:HD23	1:D:334[B]:LEU:HA	1.82	0.41
1:F:296:LYS:CE	1:F:349:SER:O	2.69	0.41
1:E:21:LYS:HG3	4:E:842:HOH:O	2.20	0.41
1:H:12:HIS:CE1	4:H:654:HOH:O	2.74	0.40
1:A:101:THR:HG21	1:E:242:ARG:NH2	2.35	0.40
1:F:3:VAL:HG12	4:F:818:HOH:O	2.20	0.40
1:F:403:GLU:HG3	4:F:814:HOH:O	2.20	0.40
1:B:190:MET:HB3	1:B:191:PRO:HD3	2.03	0.40
1:E:219[B]:THR:HG22	1:E:354:MET:HE1	2.04	0.40
1:D:241[B]:SER:OG	1:F:98:GLU:OE1	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	408/428 (95%)	401 (98%)	7 (2%)	0	100	100
1	B	415/428 (97%)	409 (99%)	6 (1%)	0	100	100
1	C	414/428 (97%)	407 (98%)	7 (2%)	0	100	100
1	D	416/428 (97%)	410 (99%)	6 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	416/428 (97%)	408 (98%)	8 (2%)	0	100	100
1	F	408/428 (95%)	401 (98%)	7 (2%)	0	100	100
1	G	411/428 (96%)	403 (98%)	8 (2%)	0	100	100
1	H	410/428 (96%)	402 (98%)	8 (2%)	0	100	100
All	All	3298/3424 (96%)	3241 (98%)	57 (2%)	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	353/365 (97%)	352 (100%)	1 (0%)	86	82
1	B	360/365 (99%)	355 (99%)	5 (1%)	59	41
1	C	359/365 (98%)	354 (99%)	5 (1%)	59	41
1	D	361/365 (99%)	359 (99%)	2 (1%)	78	71
1	E	361/365 (99%)	354 (98%)	7 (2%)	50	28
1	F	353/365 (97%)	353 (100%)	0	100	100
1	G	356/365 (98%)	356 (100%)	0	100	100
1	H	355/365 (97%)	352 (99%)	3 (1%)	73	64
All	All	2858/2920 (98%)	2835 (99%)	23 (1%)	78	64

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	317	LYS
1	B	48	GLN
1	B	207[A]	MET
1	B	207[B]	MET
1	B	207[C]	MET
1	B	406	LYS

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Mol	Chain	Res	Type
1	C	27[A]	LYS
1	C	27[B]	LYS
1	C	28	LEU
1	C	33	LYS
1	C	406	LYS
1	D	49[A]	GLN
1	D	49[B]	GLN
1	H	74	LEU
1	H	155	LYS
1	H	406	LYS
1	E	21	LYS
1	E	155[A]	LYS
1	E	155[B]	LYS
1	E	213[A]	THR
1	E	213[B]	THR
1	E	334	LEU
1	E	406	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	HIS
1	A	211	ASN
1	A	284	GLN
1	B	48	GLN
1	B	211	ASN
1	B	252	GLN
1	B	284	GLN
1	C	324	GLN
1	C	343	GLN
1	D	284	GLN
1	D	343	GLN
1	F	166	HIS
1	F	211	ASN
1	F	284	GLN
1	F	324	GLN
1	F	343	GLN
1	F	348	GLN
1	G	166	HIS
1	G	211	ASN
1	G	348	GLN
1	H	211	ASN

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Mol	Chain	Res	Type
1	H	284	GLN
1	H	343	GLN
1	E	284	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	EDO	D	503	-	3,3,3	0.38	0	2,2,2	0.20	0
3	ACT	D	502	-	3,3,3	1.01	0	3,3,3	0.88	0
2	EDO	C	501	-	3,3,3	0.56	0	2,2,2	0.37	0
3	ACT	F	501	-	3,3,3	0.97	0	3,3,3	0.92	0
3	ACT	D	501	-	3,3,3	1.28	0	3,3,3	0.68	0
3	ACT	E	601	-	3,3,3	1.07	0	3,3,3	0.39	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
2	EDO	D	503	-	-	0/1/1/1	-
2	EDO	C	501	-	-	0/1/1/1	-

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.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	502	ACT	1	0
3	E	601	ACT	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 [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	404/428 (94%)	-0.99	0 100 100	9, 20, 37, 54	6 (1%)
1	B	405/428 (94%)	-1.03	0 100 100	6, 19, 30, 46	11 (2%)
1	C	404/428 (94%)	-1.00	0 100 100	10, 20, 33, 48	12 (2%)
1	D	405/428 (94%)	-1.09	0 100 100	8, 17, 30, 45	12 (2%)
1	E	405/428 (94%)	-0.98	0 100 100	8, 20, 33, 53	13 (3%)
1	F	405/428 (94%)	-1.05	0 100 100	10, 18, 30, 51	5 (1%)
1	G	404/428 (94%)	-0.99	0 100 100	9, 21, 32, 40	9 (2%)
1	H	404/428 (94%)	-0.88	0 100 100	12, 24, 40, 52	8 (1%)
All	All	3236/3424 (94%)	-1.00	0 100 100	6, 20, 33, 54	76 (2%)

There are no RSRZ outliers to report.

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	ACT	F	501	4/4	0.97	0.07	26,35,35,35	0
2	EDO	D	503	4/4	0.98	0.05	28,29,29,30	0
3	ACT	D	502	4/4	0.98	0.06	31,33,34,34	0
2	EDO	C	501	4/4	0.98	0.06	26,30,30,33	0
3	ACT	D	501	4/4	0.99	0.05	26,31,32,33	0
3	ACT	E	601	4/4	0.99	0.05	20,27,29,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.