



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2025 – 12:11 PM JST

PDB ID : 9KD1 / pdb_00009kd1
Title : Crystal structure of Bacteroides ovatus DhuD responsible for metabolism of glycosaminoglycan
Authors : Takase, R.; Kouda, Y.; Mikami, B.; Hashimoto, W.
Deposited on : 2024-11-02
Resolution : 2.09 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

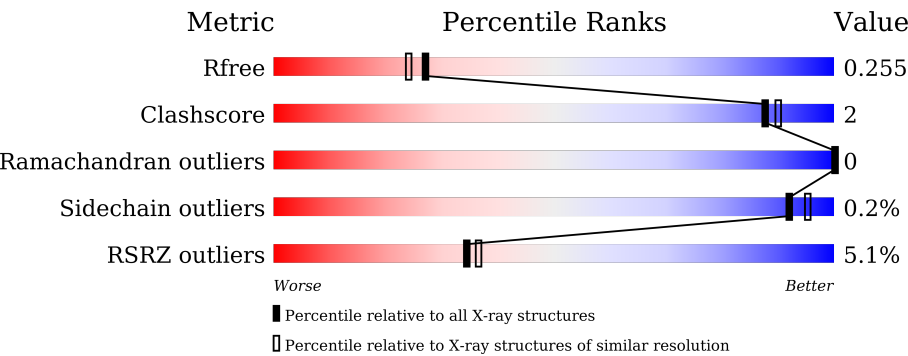
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	275	<div><div>5%</div><div><div></div><div>88%</div><div>6%</div><div>6%</div></div></div>
1	B	275	<div><div>3%</div><div><div></div><div>91%</div><div>•</div><div>5%</div></div></div>
1	C	275	<div><div>4%</div><div><div></div><div>87%</div><div>7%</div><div>6%</div></div></div>
1	D	275	<div><div>3%</div><div><div></div><div>92%</div><div>•</div><div>•</div></div></div>
1	E	275	<div><div>6%</div><div><div></div><div>90%</div><div>7%</div><div>•</div></div></div>
1	F	275	<div><div>3%</div><div><div></div><div>90%</div><div>•</div><div>6%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	275	<div><div></div><div>6%</div><div>89%</div><div>5%</div><div>5%</div></div>
1	H	275	<div><div></div><div>8%</div><div>88%</div><div>6%</div><div>6%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16357 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 Oxidoreductase, short chain dehydrogenase/reductase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1926	1224	327	359	16			
1	B	261	Total	C	N	O	S	0	0	0
			1952	1239	333	364	16			
1	C	258	Total	C	N	O	S	0	0	0
			1927	1224	327	361	15			
1	D	265	Total	C	N	O	S	0	0	0
			1977	1252	338	372	15			
1	E	266	Total	C	N	O	S	0	0	0
			1985	1257	339	373	16			
1	F	258	Total	C	N	O	S	0	0	0
			1927	1224	327	361	15			
1	G	260	Total	C	N	O	S	0	0	0
			1946	1236	332	363	15			
1	H	259	Total	C	N	O	S	0	0	0
			1937	1231	330	361	15			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	268	LEU	-	expression tag	UNP A0AAN3ACT3
A	269	GLU	-	expression tag	UNP A0AAN3ACT3
A	270	HIS	-	expression tag	UNP A0AAN3ACT3
A	271	HIS	-	expression tag	UNP A0AAN3ACT3
A	272	HIS	-	expression tag	UNP A0AAN3ACT3
A	273	HIS	-	expression tag	UNP A0AAN3ACT3
A	274	HIS	-	expression tag	UNP A0AAN3ACT3
A	275	HIS	-	expression tag	UNP A0AAN3ACT3
B	268	LEU	-	expression tag	UNP A0AAN3ACT3
B	269	GLU	-	expression tag	UNP A0AAN3ACT3
B	270	HIS	-	expression tag	UNP A0AAN3ACT3
B	271	HIS	-	expression tag	UNP A0AAN3ACT3

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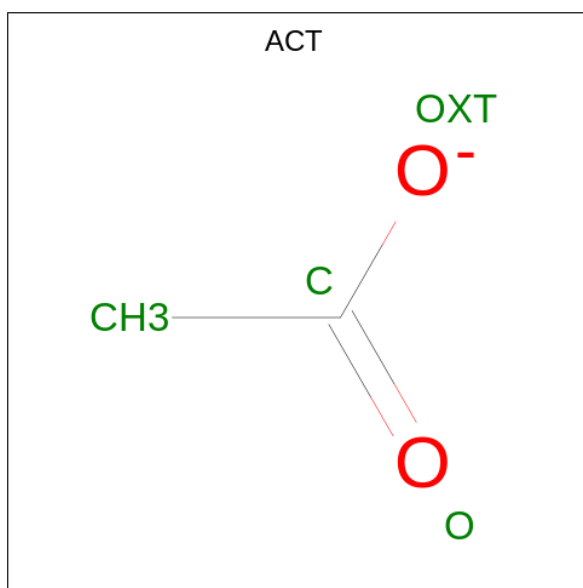
Chain	Residue	Modelled	Actual	Comment	Reference
B	272	HIS	-	expression tag	UNP A0AAN3ACT3
B	273	HIS	-	expression tag	UNP A0AAN3ACT3
B	274	HIS	-	expression tag	UNP A0AAN3ACT3
B	275	HIS	-	expression tag	UNP A0AAN3ACT3
C	268	LEU	-	expression tag	UNP A0AAN3ACT3
C	269	GLU	-	expression tag	UNP A0AAN3ACT3
C	270	HIS	-	expression tag	UNP A0AAN3ACT3
C	271	HIS	-	expression tag	UNP A0AAN3ACT3
C	272	HIS	-	expression tag	UNP A0AAN3ACT3
C	273	HIS	-	expression tag	UNP A0AAN3ACT3
C	274	HIS	-	expression tag	UNP A0AAN3ACT3
C	275	HIS	-	expression tag	UNP A0AAN3ACT3
D	268	LEU	-	expression tag	UNP A0AAN3ACT3
D	269	GLU	-	expression tag	UNP A0AAN3ACT3
D	270	HIS	-	expression tag	UNP A0AAN3ACT3
D	271	HIS	-	expression tag	UNP A0AAN3ACT3
D	272	HIS	-	expression tag	UNP A0AAN3ACT3
D	273	HIS	-	expression tag	UNP A0AAN3ACT3
D	274	HIS	-	expression tag	UNP A0AAN3ACT3
D	275	HIS	-	expression tag	UNP A0AAN3ACT3
E	268	LEU	-	expression tag	UNP A0AAN3ACT3
E	269	GLU	-	expression tag	UNP A0AAN3ACT3
E	270	HIS	-	expression tag	UNP A0AAN3ACT3
E	271	HIS	-	expression tag	UNP A0AAN3ACT3
E	272	HIS	-	expression tag	UNP A0AAN3ACT3
E	273	HIS	-	expression tag	UNP A0AAN3ACT3
E	274	HIS	-	expression tag	UNP A0AAN3ACT3
E	275	HIS	-	expression tag	UNP A0AAN3ACT3
F	268	LEU	-	expression tag	UNP A0AAN3ACT3
F	269	GLU	-	expression tag	UNP A0AAN3ACT3
F	270	HIS	-	expression tag	UNP A0AAN3ACT3
F	271	HIS	-	expression tag	UNP A0AAN3ACT3
F	272	HIS	-	expression tag	UNP A0AAN3ACT3
F	273	HIS	-	expression tag	UNP A0AAN3ACT3
F	274	HIS	-	expression tag	UNP A0AAN3ACT3
F	275	HIS	-	expression tag	UNP A0AAN3ACT3
G	268	LEU	-	expression tag	UNP A0AAN3ACT3
G	269	GLU	-	expression tag	UNP A0AAN3ACT3
G	270	HIS	-	expression tag	UNP A0AAN3ACT3
G	271	HIS	-	expression tag	UNP A0AAN3ACT3
G	272	HIS	-	expression tag	UNP A0AAN3ACT3
G	273	HIS	-	expression tag	UNP A0AAN3ACT3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	274	HIS	-	expression tag	UNP A0AAN3ACT3
G	275	HIS	-	expression tag	UNP A0AAN3ACT3
H	268	LEU	-	expression tag	UNP A0AAN3ACT3
H	269	GLU	-	expression tag	UNP A0AAN3ACT3
H	270	HIS	-	expression tag	UNP A0AAN3ACT3
H	271	HIS	-	expression tag	UNP A0AAN3ACT3
H	272	HIS	-	expression tag	UNP A0AAN3ACT3
H	273	HIS	-	expression tag	UNP A0AAN3ACT3
H	274	HIS	-	expression tag	UNP A0AAN3ACT3
H	275	HIS	-	expression tag	UNP A0AAN3ACT3

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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


- Molecule 3 is water.

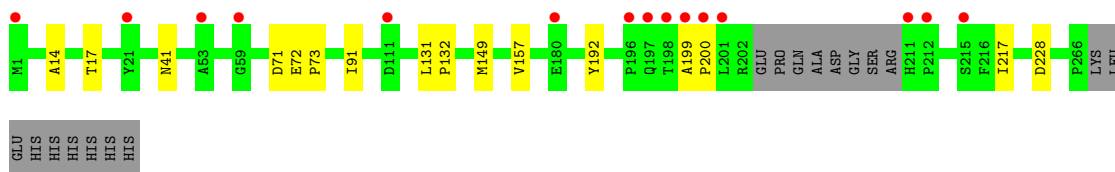
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	106	Total 106	O 106	0	0
3	B	92	Total 92	O 92	0	0
3	C	99	Total 99	O 99	0	0
3	D	104	Total 104	O 104	0	0
3	E	97	Total 97	O 97	0	0
3	F	118	Total 118	O 118	0	0
3	G	80	Total 80	O 80	0	0
3	H	68	Total 68	O 68	0	0

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.

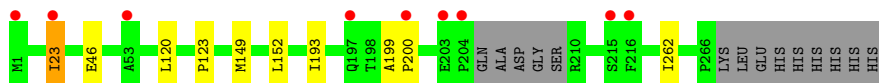
- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family protein

Chain A: 




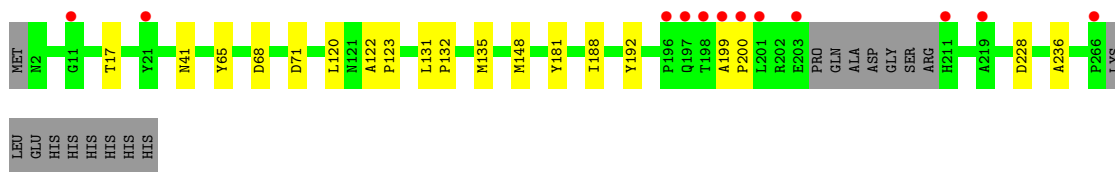
- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family protein

Chain B: 

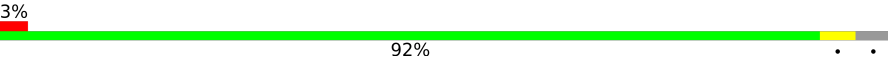


- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family protein

Chain C: 




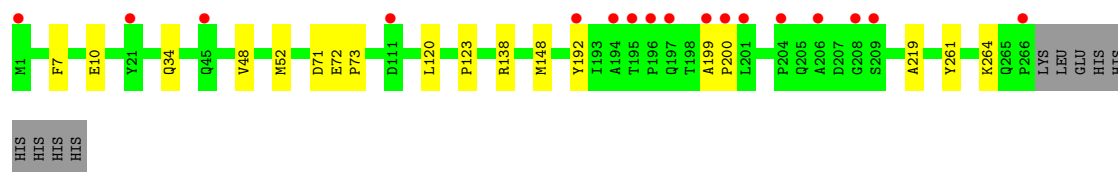
- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family protein

Chain D: 

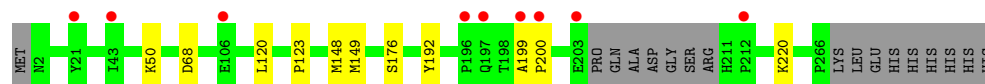
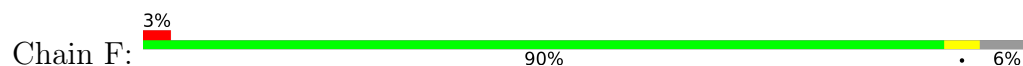


- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family protein

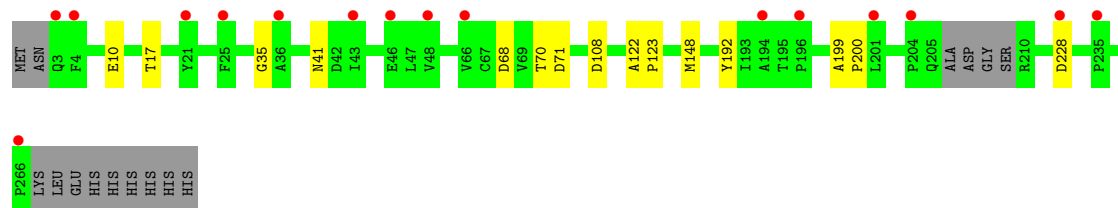
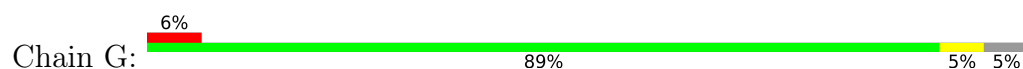
Chain E: 



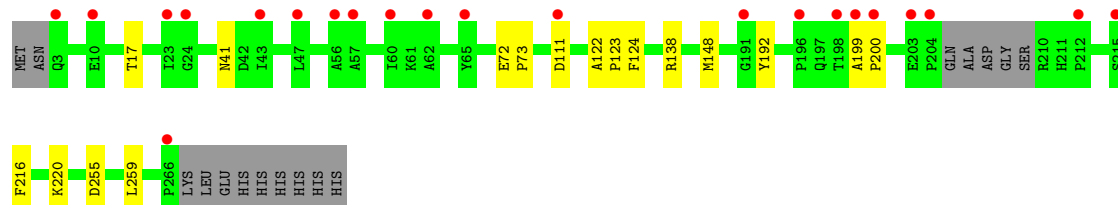
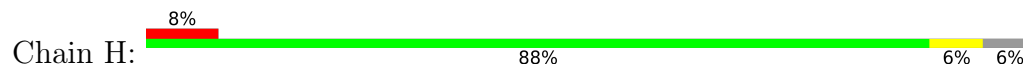
- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family protein



- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family protein



- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.64Å 75.45Å 102.07Å 97.69° 96.42° 95.33°	Depositor
Resolution (Å)	40.99 – 2.09 40.99 – 2.09	Depositor EDS
% Data completeness (in resolution range)	96.7 (40.99-2.09) 97.2 (40.99-2.09)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.208 , 0.252 0.215 , 0.255	Depositor DCC
R_{free} test set	5884 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.679	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16357	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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: 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	0.50	0/1961	0.89	2/2655 (0.1%)
1	B	0.51	0/1987	0.90	0/2689
1	C	0.50	0/1962	0.89	4/2657 (0.2%)
1	D	0.51	0/2014	0.88	1/2729 (0.0%)
1	E	0.51	0/2022	0.91	1/2739 (0.0%)
1	F	0.51	0/1962	0.91	1/2657 (0.0%)
1	G	0.50	0/1982	0.92	3/2684 (0.1%)
1	H	0.51	0/1973	0.89	1/2672 (0.0%)
All	All	0.51	0/15863	0.90	13/21482 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	ASP	CA-CB-CG	6.09	118.69	112.60
1	D	71	ASP	CA-CB-CG	5.98	118.58	112.60
1	F	68	ASP	CA-CB-CG	5.54	118.14	112.60
1	C	71	ASP	CA-CB-CG	5.33	117.93	112.60
1	G	71	ASP	CA-CB-CG	5.29	117.89	112.60
1	C	68	ASP	CA-CB-CG	5.27	117.87	112.60
1	C	228	ASP	CB-CA-C	5.25	116.98	109.26
1	E	71	ASP	CA-CB-CG	5.24	117.84	112.60
1	H	111	ASP	CA-CB-CG	5.23	117.83	112.60
1	G	228	ASP	CA-CB-CG	5.23	117.83	112.60
1	C	228	ASP	CA-CB-CG	5.18	117.78	112.60
1	G	108	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	228	ASP	CA-CB-CG	5.13	117.73	112.60

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	1926	0	1934	7	0
1	B	1952	0	1956	5	0
1	C	1927	0	1928	9	0
1	D	1977	0	1974	6	0
1	E	1985	0	1986	10	0
1	F	1927	0	1928	8	0
1	G	1946	0	1950	7	0
1	H	1937	0	1942	8	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
2	D	4	0	3	1	0
2	E	4	0	3	0	0
3	A	106	0	0	0	0
3	B	92	0	0	0	0
3	C	99	0	0	0	0
3	D	104	0	0	0	0
3	E	97	0	0	1	0
3	F	118	0	0	1	0
3	G	80	0	0	0	0
3	H	68	0	0	1	0
All	All	16357	0	15610	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 2.

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:B:23:ILE:HD11	1:B:193:ILE:HG21	1.84	0.58
1:A:199:ALA:N	1:A:200:PRO:HD2	2.19	0.57
1:D:135:MET:O	1:D:138:ARG:NH1	2.38	0.56
1:E:7:PHE:O	1:E:34:GLN:NE2	2.40	0.52
1:G:68:ASP:OD1	1:G:70:THR:OG1	2.28	0.51
1:H:199:ALA:N	1:H:200:PRO:CD	2.75	0.50
1:G:17:THR:HA	1:G:41:ASN:OD1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:LEU:C	1:B:123:PRO:HD2	2.38	0.49
1:E:138:ARG:NE	3:E:401:HOH:O	2.45	0.48
1:H:216:PHE:CZ	1:H:220:LYS:HD2	2.48	0.48
1:H:138:ARG:NH2	3:H:302:HOH:O	2.43	0.48
1:D:90:ASP:OD1	1:D:137:LYS:HE3	2.13	0.48
1:E:199:ALA:N	1:E:200:PRO:CD	2.77	0.48
1:E:10:GLU:CD	1:E:10:GLU:C	2.81	0.47
1:A:17:THR:HA	1:A:41:ASN:OD1	2.14	0.47
1:B:199:ALA:N	1:B:200:PRO:CD	2.79	0.46
1:D:17:THR:HA	1:D:41:ASN:OD1	2.16	0.46
1:F:148:MET:HE1	1:F:192:TYR:CE2	2.51	0.46
1:E:120:LEU:C	1:E:123:PRO:HD2	2.41	0.45
1:F:148:MET:C	1:F:149:MET:HE2	2.41	0.45
1:G:148:MET:HE1	1:G:192:TYR:CE2	2.51	0.45
1:H:122:ALA:HB3	1:H:123:PRO:HD3	1.99	0.45
1:H:148:MET:HE1	1:H:192:TYR:CE2	2.52	0.45
1:E:48:VAL:O	1:E:52:MET:HG2	2.17	0.45
1:E:261:TYR:CD1	1:F:176:SER:HB3	2.52	0.44
1:F:120:LEU:C	1:F:123:PRO:HD2	2.42	0.44
1:G:199:ALA:N	1:G:200:PRO:CD	2.80	0.44
1:A:131:LEU:N	1:A:132:PRO:CD	2.81	0.44
1:A:149:MET:HE2	1:A:157:VAL:HG21	1.99	0.44
1:C:199:ALA:N	1:C:200:PRO:CD	2.80	0.43
1:C:188:ILE:HD11	1:C:236:ALA:HA	2.00	0.43
1:G:122:ALA:HB3	1:G:123:PRO:HD3	2.00	0.43
1:F:199:ALA:N	1:F:200:PRO:CD	2.81	0.43
1:A:14:ALA:HA	1:A:91:ILE:O	2.18	0.43
1:F:149:MET:HE2	1:F:149:MET:N	2.34	0.43
1:C:135:MET:HE3	1:C:181:TYR:CZ	2.54	0.43
1:E:72:GLU:HB3	1:E:73:PRO:HD3	2.01	0.43
1:H:255:ASP:OD2	1:H:259:LEU:HG	2.19	0.42
1:H:72:GLU:HB3	1:H:73:PRO:HD3	2.01	0.42
1:D:250:HIS:ND1	2:D:301:ACT:H3	2.35	0.42
1:C:120:LEU:C	1:C:123:PRO:HD2	2.45	0.42
1:G:10:GLU:HA	1:G:35:GLY:O	2.20	0.42
1:C:17:THR:HA	1:C:41:ASN:OD1	2.20	0.42
1:C:122:ALA:HB3	1:C:123:PRO:HD3	2.02	0.42
1:B:262:ILE:O	1:F:220:LYS:NZ	2.35	0.42
1:E:148:MET:HE1	1:E:192:TYR:CE2	2.55	0.41
1:A:72:GLU:HB3	1:A:73:PRO:HD3	2.03	0.41
1:C:131:LEU:N	1:C:132:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:ASN:HA	1:C:65:TYR:O	2.20	0.41
1:A:192:TYR:CD2	1:A:217:ILE:HD12	2.56	0.41
1:F:50:LYS:NZ	3:F:308:HOH:O	2.53	0.41
1:E:219:ALA:HB1	1:E:264:LYS:HD3	2.03	0.41
1:B:149:MET:HA	1:B:152:LEU:O	2.21	0.41
1:C:148:MET:HE1	1:C:192:TYR:CE2	2.56	0.41
1:D:122:ALA:HB3	1:D:123:PRO:HD3	2.03	0.41
1:D:216:PHE:CZ	1:D:220:LYS:HD2	2.56	0.41
1:G:68:ASP:OD1	1:G:68:ASP:C	2.64	0.41
1:H:17:THR:HA	1:H:41:ASN:OD1	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	254/275 (92%)	246 (97%)	8 (3%)	0	100	100
1	B	257/275 (94%)	249 (97%)	8 (3%)	0	100	100
1	C	254/275 (92%)	246 (97%)	8 (3%)	0	100	100
1	D	263/275 (96%)	252 (96%)	11 (4%)	0	100	100
1	E	264/275 (96%)	257 (97%)	7 (3%)	0	100	100
1	F	254/275 (92%)	247 (97%)	7 (3%)	0	100	100
1	G	256/275 (93%)	245 (96%)	11 (4%)	0	100	100
1	H	255/275 (93%)	246 (96%)	9 (4%)	0	100	100
All	All	2057/2200 (94%)	1988 (97%)	69 (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	197/212 (93%)	197 (100%)	0	100	100
1	B	200/212 (94%)	198 (99%)	2 (1%)	73	79
1	C	197/212 (93%)	197 (100%)	0	100	100
1	D	202/212 (95%)	202 (100%)	0	100	100
1	E	203/212 (96%)	203 (100%)	0	100	100
1	F	197/212 (93%)	197 (100%)	0	100	100
1	G	199/212 (94%)	199 (100%)	0	100	100
1	H	198/212 (93%)	197 (100%)	1 (0%)	86	91
All	All	1593/1696 (94%)	1590 (100%)	3 (0%)	92	95

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

Mol	Chain	Res	Type
1	B	23	ILE
1	B	46	GLU
1	H	124	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	63	HIS
1	B	94	ASN
1	C	94	ASN
1	D	63	HIS
1	E	63	HIS
1	G	205	GLN
1	H	94	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	ACT	E	301	-	3,3,3	0.90	0	3,3,3	0.88	0
2	ACT	D	301	-	3,3,3	0.92	0	3,3,3	0.63	0
2	ACT	B	301	-	3,3,3	1.03	0	3,3,3	0.88	0
2	ACT	A	301	-	3,3,3	1.03	0	3,3,3	0.88	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	ACT	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	258/275 (93%)	0.40	15 (5%) 30 32	8, 15, 35, 53	0
1	B	261/275 (94%)	0.31	9 (3%) 48 50	9, 16, 29, 47	0
1	C	258/275 (93%)	0.36	12 (4%) 37 39	10, 16, 33, 69	0
1	D	265/275 (96%)	0.31	7 (2%) 57 59	11, 17, 29, 38	0
1	E	266/275 (96%)	0.55	17 (6%) 27 29	10, 16, 40, 54	0
1	F	258/275 (93%)	0.43	9 (3%) 47 49	9, 16, 31, 54	0
1	G	260/275 (94%)	0.72	16 (6%) 28 30	12, 21, 34, 47	0
1	H	259/275 (94%)	0.85	22 (8%) 18 19	13, 23, 40, 48	0
All	All	2085/2200 (94%)	0.49	107 (5%) 34 36	8, 17, 35, 69	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	200	PRO	4.5
1	E	1	MET	4.2
1	A	201	LEU	4.2
1	A	200	PRO	4.2
1	A	1	MET	4.2
1	C	198	THR	4.1
1	F	106	GLU	4.0
1	C	200	PRO	3.9
1	F	199	ALA	3.9
1	H	204	PRO	3.9
1	H	212	PRO	3.8
1	A	211	HIS	3.8
1	G	46	GLU	3.7
1	H	57	ALA	3.7
1	C	266	PRO	3.6
1	B	1	MET	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	201	LEU	3.6
1	C	199	ALA	3.5
1	E	199	ALA	3.5
1	F	196	PRO	3.4
1	H	23	ILE	3.4
1	C	21	TYR	3.4
1	H	199	ALA	3.3
1	A	199	ALA	3.3
1	G	228	ASP	3.3
1	C	197	GLN	3.3
1	G	196	PRO	3.2
1	E	111	ASP	3.1
1	A	212	PRO	3.0
1	F	21	TYR	3.0
1	H	10	GLU	2.9
1	D	208	GLY	2.9
1	C	203	GLU	2.9
1	F	200	PRO	2.8
1	H	62	ALA	2.8
1	G	21	TYR	2.8
1	A	111	ASP	2.8
1	B	204	PRO	2.7
1	G	201	LEU	2.7
1	H	200	PRO	2.7
1	A	215	SER	2.7
1	E	194	ALA	2.7
1	G	204	PRO	2.7
1	H	198	THR	2.7
1	G	3	GLN	2.6
1	G	266	PRO	2.6
1	H	215	SER	2.6
1	G	194	ALA	2.6
1	G	43	ILE	2.6
1	H	60	ILE	2.6
1	F	197	GLN	2.5
1	F	203	GLU	2.5
1	F	43	ILE	2.5
1	G	36	ALA	2.5
1	A	196	PRO	2.4
1	D	21	TYR	2.4
1	E	208	GLY	2.4
1	E	197	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	53	ALA	2.4
1	E	195	THR	2.4
1	G	235	PRO	2.4
1	C	11	GLY	2.4
1	E	206	ALA	2.4
1	H	191	GLY	2.4
1	D	46	GLU	2.3
1	C	211	HIS	2.3
1	H	266	PRO	2.3
1	A	197	GLN	2.3
1	E	201	LEU	2.3
1	H	3	GLN	2.3
1	D	197	GLN	2.3
1	B	200	PRO	2.3
1	E	196	PRO	2.3
1	B	203	GLU	2.3
1	B	197	GLN	2.3
1	G	25	PHE	2.2
1	E	192	TYR	2.2
1	A	180	GLU	2.2
1	H	111	ASP	2.2
1	H	43	ILE	2.2
1	A	198	THR	2.2
1	B	216	PHE	2.2
1	B	23	ILE	2.2
1	G	4	PHE	2.1
1	B	215	SER	2.1
1	D	88	THR	2.1
1	D	266	PRO	2.1
1	H	24	GLY	2.1
1	E	45	GLN	2.1
1	G	66	VAL	2.1
1	H	47	LEU	2.1
1	B	53	ALA	2.1
1	C	219	ALA	2.1
1	C	196	PRO	2.1
1	G	48	VAL	2.1
1	D	138	ARG	2.1
1	E	209	SER	2.1
1	A	59	GLY	2.0
1	E	204	PRO	2.0
1	E	266	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	196	PRO	2.0
1	H	203	GLU	2.0
1	A	21	TYR	2.0
1	F	212	PRO	2.0
1	H	56	ALA	2.0
1	E	21	TYR	2.0
1	H	65	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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(Å ²)	Q<0.9
2	ACT	A	301	4/4	0.58	0.24	31,32,34,36	0
2	ACT	D	301	4/4	0.62	0.23	17,18,19,22	0
2	ACT	B	301	4/4	0.66	0.18	24,24,25,28	0
2	ACT	E	301	4/4	0.75	0.13	28,28,29,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.