



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:01 PM UTC

PDB ID : 4PN3 / pdb_00004pn3
Title : Crystal structure of 3-hydroxyacyl-CoA-dehydrogenase from Brucella melitensis
Authors : Lukacs, C.M.; Abendroth, J.; Edwards, T.E.; Lorimer, D.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2014-05-22
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 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

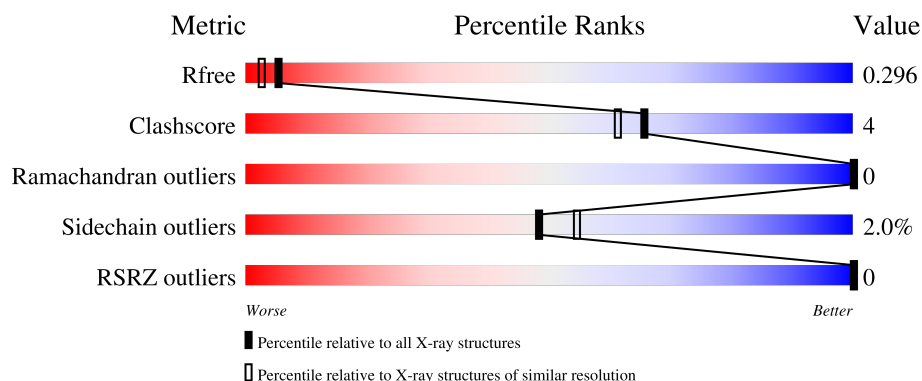
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (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 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	263	 90% 8% ..
1	B	263	 90% 8% ..
1	C	263	 92% 7% .
1	D	263	 87% 7% 5%
1	E	263	 92% 5% ..

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Mol	Chain	Length	Quality of chain
1	F	263	 90% 6%
1	G	263	 91% 6%
1	H	263	 87% 8% 6%

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
2	TRS	F	301	-	X	-	-
2	TRS	G	301	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14988 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 3-hydroxyacyl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	2	0
			1867	1164	342	348	13			
1	B	260	Total	C	N	O	S	0	0	0
			1845	1149	338	347	11			
1	C	259	Total	C	N	O	S	0	0	0
			1811	1131	328	342	10			
1	D	249	Total	C	N	O	S	0	0	0
			1759	1098	322	330	9			
1	E	257	Total	C	N	O	S	0	0	0
			1829	1141	332	345	11			
1	F	254	Total	C	N	O	S	0	0	0
			1803	1124	332	338	9			
1	G	256	Total	C	N	O	S	0	0	0
			1795	1120	324	342	9			
1	H	248	Total	C	N	O	S	0	0	0
			1750	1091	321	329	9			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP N7K0F6
A	-6	ALA	-	expression tag	UNP N7K0F6
A	-5	HIS	-	expression tag	UNP N7K0F6
A	-4	HIS	-	expression tag	UNP N7K0F6
A	-3	HIS	-	expression tag	UNP N7K0F6
A	-2	HIS	-	expression tag	UNP N7K0F6
A	-1	HIS	-	expression tag	UNP N7K0F6
A	0	HIS	-	expression tag	UNP N7K0F6
B	-7	MET	-	initiating methionine	UNP N7K0F6
B	-6	ALA	-	expression tag	UNP N7K0F6
B	-5	HIS	-	expression tag	UNP N7K0F6
B	-4	HIS	-	expression tag	UNP N7K0F6
B	-3	HIS	-	expression tag	UNP N7K0F6

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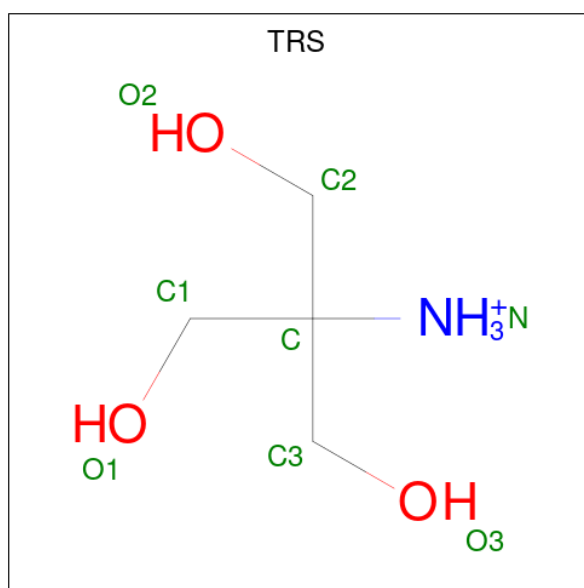
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP N7K0F6
B	-1	HIS	-	expression tag	UNP N7K0F6
B	0	HIS	-	expression tag	UNP N7K0F6
C	-7	MET	-	initiating methionine	UNP N7K0F6
C	-6	ALA	-	expression tag	UNP N7K0F6
C	-5	HIS	-	expression tag	UNP N7K0F6
C	-4	HIS	-	expression tag	UNP N7K0F6
C	-3	HIS	-	expression tag	UNP N7K0F6
C	-2	HIS	-	expression tag	UNP N7K0F6
C	-1	HIS	-	expression tag	UNP N7K0F6
C	0	HIS	-	expression tag	UNP N7K0F6
D	-7	MET	-	initiating methionine	UNP N7K0F6
D	-6	ALA	-	expression tag	UNP N7K0F6
D	-5	HIS	-	expression tag	UNP N7K0F6
D	-4	HIS	-	expression tag	UNP N7K0F6
D	-3	HIS	-	expression tag	UNP N7K0F6
D	-2	HIS	-	expression tag	UNP N7K0F6
D	-1	HIS	-	expression tag	UNP N7K0F6
D	0	HIS	-	expression tag	UNP N7K0F6
E	-7	MET	-	initiating methionine	UNP N7K0F6
E	-6	ALA	-	expression tag	UNP N7K0F6
E	-5	HIS	-	expression tag	UNP N7K0F6
E	-4	HIS	-	expression tag	UNP N7K0F6
E	-3	HIS	-	expression tag	UNP N7K0F6
E	-2	HIS	-	expression tag	UNP N7K0F6
E	-1	HIS	-	expression tag	UNP N7K0F6
E	0	HIS	-	expression tag	UNP N7K0F6
F	-7	MET	-	initiating methionine	UNP N7K0F6
F	-6	ALA	-	expression tag	UNP N7K0F6
F	-5	HIS	-	expression tag	UNP N7K0F6
F	-4	HIS	-	expression tag	UNP N7K0F6
F	-3	HIS	-	expression tag	UNP N7K0F6
F	-2	HIS	-	expression tag	UNP N7K0F6
F	-1	HIS	-	expression tag	UNP N7K0F6
F	0	HIS	-	expression tag	UNP N7K0F6
G	-7	MET	-	initiating methionine	UNP N7K0F6
G	-6	ALA	-	expression tag	UNP N7K0F6
G	-5	HIS	-	expression tag	UNP N7K0F6
G	-4	HIS	-	expression tag	UNP N7K0F6
G	-3	HIS	-	expression tag	UNP N7K0F6
G	-2	HIS	-	expression tag	UNP N7K0F6
G	-1	HIS	-	expression tag	UNP N7K0F6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP N7K0F6
H	-7	MET	-	initiating methionine	UNP N7K0F6
H	-6	ALA	-	expression tag	UNP N7K0F6
H	-5	HIS	-	expression tag	UNP N7K0F6
H	-4	HIS	-	expression tag	UNP N7K0F6
H	-3	HIS	-	expression tag	UNP N7K0F6
H	-2	HIS	-	expression tag	UNP N7K0F6
H	-1	HIS	-	expression tag	UNP N7K0F6
H	0	HIS	-	expression tag	UNP N7K0F6

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			8	4	1	3		
2	D	1	Total	C	N	O	0	0
			8	4	1	3		
2	F	1	Total	C	N	O	0	0
			8	4	1	3		
2	G	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	75	Total 75	O 75	0	0
3	B	56	Total 56	O 56	0	0
3	C	49	Total 49	O 49	0	0
3	D	71	Total 71	O 71	0	0
3	E	83	Total 83	O 83	0	0
3	F	64	Total 64	O 64	0	0
3	G	38	Total 38	O 38	0	0
3	H	61	Total 61	O 61	0	0

3 Residue-property plots [i](#)

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

- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

Chain A: 



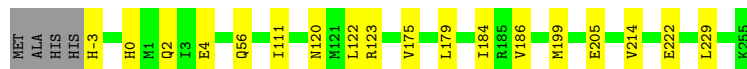
- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

Chain B: 



- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

Chain C: 



- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

Chain D: 



- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

Chain E: 

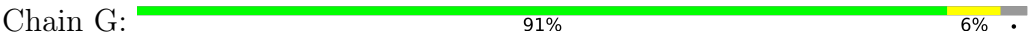


- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

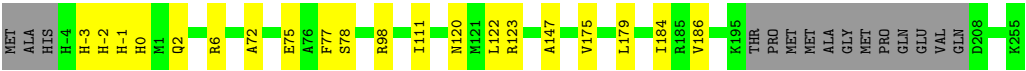
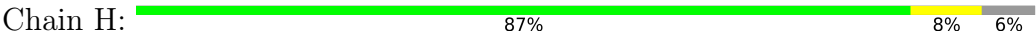
Chain F: 



• Molecule 1: 3-hydroxyacyl-CoA dehydrogenase



• Molecule 1: 3-hydroxyacyl-CoA dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	72.84Å 72.84Å 350.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.13 – 2.15 47.13 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.8 (47.13-2.15) 97.8 (47.13-2.15)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.74 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.236 , 0.264 (Not available) , 0.296	Depositor DCC
R_{free} test set	1885 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å ²)	17.1	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 18.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.458 for h,-k,-l	Xtriage
Reported twinning fraction	0.547 for H, K, L 0.453 for K, H, -L	Depositor
Outliers	1 of 96205 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	14988	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: TRS

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.99	0/1893	1.00	1/2561 (0.0%)
1	B	0.91	2/1871 (0.1%)	1.00	5/2533 (0.2%)
1	C	0.83	1/1837 (0.1%)	0.93	0/2495
1	D	0.90	0/1783	0.99	3/2415 (0.1%)
1	E	0.94	0/1853	0.96	2/2508 (0.1%)
1	F	0.86	0/1827	0.91	0/2474
1	G	0.85	0/1818	0.91	0/2467
1	H	0.89	1/1773 (0.1%)	0.94	1/2400 (0.0%)
All	All	0.90	4/14655 (0.0%)	0.96	12/19853 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	147	ALA	N-CA	-6.03	1.42	1.46
1	B	123	ARG	CD-NE	-5.51	1.38	1.46
1	C	214	VAL	N-CA	5.39	1.50	1.46
1	H	147	ALA	CA-C	-5.05	1.50	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	-2	HIS	N-CA-C	7.71	119.32	111.07
1	B	123	ARG	CD-NE-CZ	-7.16	114.38	124.40
1	B	-2	HIS	N-CA-C	7.15	118.72	111.07
1	B	67	LYS	CB-CA-C	-7.03	99.85	110.88
1	D	195	LYS	N-CA-C	5.99	118.44	110.53
1	D	140	ARG	NE-CZ-NH2	5.83	124.44	119.20
1	E	60	VAL	CA-CB-CG2	5.83	120.30	110.40
1	D	6	ARG	CA-CB-CG	5.49	125.07	114.10
1	A	70	ILE	N-CA-C	-5.46	105.18	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	6	ARG	N-CA-CB	5.26	118.28	110.29
1	B	123	ARG	CG-CD-NE	-5.25	100.44	112.00
1	B	60	VAL	CA-CB-CG2	5.21	119.25	110.40

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	1867	0	1871	16	0
1	B	1845	0	1834	17	0
1	C	1811	0	1780	12	0
1	D	1759	0	1745	14	0
1	E	1829	0	1840	12	0
1	F	1803	0	1794	16	0
1	G	1795	0	1782	12	0
1	H	1750	0	1733	17	0
2	B	8	0	12	1	0
2	D	8	0	12	1	0
2	F	8	0	12	0	0
2	G	8	0	12	1	0
3	A	75	0	0	8	0
3	B	56	0	0	5	0
3	C	49	0	0	2	0
3	D	71	0	0	5	0
3	E	83	0	0	6	0
3	F	64	0	0	6	0
3	G	38	0	0	2	0
3	H	61	0	0	4	0
All	All	14988	0	14427	111	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 4.

All (111) 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)
2:G:301:TRS:O1	2:G:301:TRS:O2	1.77	0.98
1:F:133:GLU:OE2	1:F:134:PRO:HD2	1.61	0.98
1:D:1:MET:HE3	3:D:455:HOH:O	1.64	0.96
1:A:207:GLN:HG2	1:A:220:LEU:HD11	1.48	0.95
1:B:120:ASN:OD1	1:B:123:ARG:NH2	2.02	0.92
1:C:2:GLN:NE2	1:C:4:GLU:OE1	2.08	0.85
1:G:222:GLU:HG3	1:H:-1:HIS:CD2	2.17	0.79
1:F:-1:HIS:O	1:F:1:MET:HE2	1.83	0.78
1:A:75:GLU:HG2	3:A:346:HOH:O	1.83	0.78
1:A:130:ALA:O	3:A:338:HOH:O	2.03	0.75
1:F:133:GLU:OE2	1:F:133:GLU:HA	1.87	0.73
1:B:200:ALA:HB3	3:B:449:HOH:O	1.89	0.72
1:B:64:THR:HG23	3:B:401:HOH:O	1.88	0.72
1:A:237:GLN:OE1	1:H:98:ARG:NH2	2.27	0.67
1:F:113:ILE:O	3:F:445:HOH:O	2.13	0.66
1:C:56:GLN:NE2	3:C:328:HOH:O	2.29	0.65
1:F:133:GLU:OE2	1:F:134:PRO:CD	2.41	0.64
1:G:214:VAL:O	3:G:420:HOH:O	2.13	0.64
1:G:68:ALA:HB3	3:G:426:HOH:O	1.97	0.64
1:E:153:ASP:OD2	3:E:311:HOH:O	2.15	0.63
1:G:89:VAL:HG12	1:G:91:PRO:HD3	1.82	0.60
3:E:313:HOH:O	1:F:238:MET:HE1	2.02	0.60
1:A:198[B]:MET:HE3	3:A:341:HOH:O	2.01	0.59
1:E:68:ALA:HA	3:E:304:HOH:O	2.01	0.58
1:F:178:GLU:HB2	3:F:454:HOH:O	2.04	0.57
1:A:158:GLN:HG2	3:A:333:HOH:O	2.04	0.57
1:A:232:HIS:HB2	3:B:443:HOH:O	2.06	0.56
3:A:362:HOH:O	1:D:100:GLY:HA2	2.06	0.56
1:C:-3:HIS:ND1	1:C:0:HIS:HB2	2.21	0.56
1:G:120:ASN:O	1:G:123:ARG:HG2	2.06	0.56
1:H:2:GLN:O	1:H:6:ARG:HD2	2.05	0.56
1:A:77:PHE:O	1:A:78:SER:OG	2.18	0.55
1:F:250:LEU:HD12	3:F:453:HOH:O	2.05	0.55
1:A:120:ASN:O	1:A:123:ARG:HG2	2.06	0.55
1:E:120:ASN:O	1:E:123:ARG:HG2	2.07	0.55
1:D:131:LYS:HG3	3:D:451:HOH:O	2.06	0.55
1:H:120:ASN:O	1:H:123:ARG:HG2	2.07	0.54
1:B:120:ASN:O	1:B:123:ARG:HG2	2.07	0.54
1:F:67:LYS:O	3:F:457:HOH:O	2.18	0.54
1:F:120:ASN:O	1:F:123:ARG:HG2	2.07	0.54
1:D:120:ASN:O	1:D:123:ARG:HG2	2.07	0.54
1:C:120:ASN:O	1:C:123:ARG:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ASN:HA	1:B:123:ARG:HD3	1.89	0.54
1:B:242:GLU:OE1	2:B:301:TRS:O2	2.24	0.53
1:D:120:ASN:HA	1:D:123:ARG:HD3	1.91	0.53
1:B:232:HIS:ND1	3:B:443:HOH:O	2.34	0.52
1:C:120:ASN:HA	1:C:123:ARG:HD3	1.92	0.52
1:F:120:ASN:HA	1:F:123:ARG:HD3	1.92	0.52
1:H:75:GLU:HB2	3:H:301:HOH:O	2.10	0.51
1:E:120:ASN:HA	1:E:123:ARG:HD3	1.93	0.51
1:H:120:ASN:HA	1:H:123:ARG:HD3	1.92	0.51
1:C:205:GLU:OE2	3:C:301:HOH:O	2.19	0.51
1:F:68:ALA:HB1	3:F:417:HOH:O	2.10	0.51
1:A:120:ASN:HA	1:A:123:ARG:HD3	1.92	0.51
1:G:120:ASN:HA	1:G:123:ARG:HD3	1.92	0.51
1:B:199:MET:HE3	1:B:207:GLN:HG2	1.92	0.50
1:D:6:ARG:HG3	1:D:81:ASP:CB	2.41	0.50
1:H:72:ALA:HB2	3:H:319:HOH:O	2.11	0.50
2:D:301:TRS:O1	2:D:301:TRS:O3	2.24	0.49
1:E:60:VAL:HG23	1:E:121:MET:HG2	1.95	0.49
1:G:75:GLU:CD	1:G:75:GLU:C	2.80	0.49
1:G:222:GLU:HG3	1:H:-1:HIS:NE2	2.27	0.49
1:H:6:ARG:NH2	3:H:302:HOH:O	2.46	0.49
1:B:199:MET:CE	1:B:207:GLN:HA	2.43	0.49
1:D:6:ARG:HG3	1:D:81:ASP:HB3	1.96	0.48
1:G:98:ARG:NH1	1:G:99:GLU:OE2	2.47	0.48
3:A:338:HOH:O	1:E:140:ARG:NH1	2.48	0.47
1:B:219:ARG:HE	1:H:98:ARG:NH2	2.12	0.47
1:A:198[B]:MET:HG2	3:A:341:HOH:O	2.15	0.47
1:F:133:GLU:OE2	1:F:133:GLU:CA	2.56	0.47
1:H:6:ARG:HH11	1:H:6:ARG:HG3	1.80	0.46
1:F:155:GLN:NE2	3:F:464:HOH:O	2.46	0.46
1:A:135:GLY:HA2	3:A:372:HOH:O	2.15	0.46
1:A:132:ASN:O	1:A:140:ARG:HD3	2.15	0.46
1:E:3:ILE:O	1:E:6:ARG:HG2	2.15	0.45
1:E:6:ARG:NH1	3:E:329:HOH:O	2.48	0.45
1:A:175:VAL:HG12	1:A:186:VAL:HG21	1.98	0.45
1:B:219:ARG:HE	1:H:98:ARG:CZ	2.30	0.45
1:F:-1:HIS:O	1:F:1:MET:CE	2.59	0.45
1:D:30:ALA:N	3:D:401:HOH:O	2.48	0.45
1:D:2:GLN:HG2	3:D:450:HOH:O	2.17	0.45
1:B:132:ASN:O	1:B:140:ARG:HD3	2.18	0.44
1:H:75:GLU:HG2	3:H:306:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:ASN:O	1:E:140:ARG:HD3	2.17	0.43
1:G:175:VAL:HG12	1:G:186:VAL:HG21	2.00	0.43
1:C:222:GLU:HG3	1:D:-1:HIS:ND1	2.33	0.43
1:E:175:VAL:HG12	1:E:186:VAL:HG21	2.00	0.43
1:E:140:ARG:NH2	3:E:374:HOH:O	2.51	0.43
1:C:175:VAL:HG12	1:C:186:VAL:HG21	2.01	0.43
1:H:175:VAL:HG12	1:H:186:VAL:HG21	2.01	0.43
1:B:60:VAL:HG23	1:B:121:MET:HG2	2.00	0.43
1:B:123:ARG:HD3	1:B:123:ARG:HH21	1.38	0.43
1:D:29:GLY:C	3:D:401:HOH:O	2.61	0.43
1:G:89:VAL:HG12	1:G:91:PRO:CD	2.49	0.43
1:H:179:LEU:HB3	1:H:184:ILE:HB	2.00	0.42
1:B:60:VAL:HG22	1:B:117:GLY:C	2.45	0.42
1:H:77:PHE:O	1:H:78:SER:HB3	2.19	0.41
1:B:175:VAL:HG12	1:B:186:VAL:HG21	2.02	0.41
1:C:-3:HIS:ND1	1:C:0:HIS:N	2.68	0.41
1:D:175:VAL:HG12	1:D:186:VAL:HG21	2.02	0.41
1:H:-3:HIS:CD2	1:H:0:HIS:HB2	2.56	0.41
1:F:179:LEU:HB3	1:F:184:ILE:HB	2.02	0.41
1:C:229:LEU:HA	1:D:232:HIS:CE1	2.55	0.41
1:C:179:LEU:HB3	1:C:184:ILE:HB	2.03	0.41
1:D:122:LEU:C	1:D:122:LEU:HD23	2.46	0.41
1:G:75:GLU:CD	1:G:75:GLU:O	2.64	0.41
1:A:196:THR:OG1	1:A:198[B]:MET:HG2	2.21	0.40
1:A:111:ILE:HD12	1:A:164:SER:HB3	2.03	0.40
1:B:253:ALA:HB2	3:B:451:HOH:O	2.21	0.40
1:C:199:MET:HE2	1:C:199:MET:HB2	1.92	0.40
1:E:57:ARG:NE	3:E:362:HOH:O	2.55	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	260/263 (99%)	252 (97%)	8 (3%)	0	100	100
1	B	258/263 (98%)	252 (98%)	6 (2%)	0	100	100
1	C	257/263 (98%)	248 (96%)	9 (4%)	0	100	100
1	D	245/263 (93%)	240 (98%)	5 (2%)	0	100	100
1	E	255/263 (97%)	249 (98%)	6 (2%)	0	100	100
1	F	250/263 (95%)	244 (98%)	6 (2%)	0	100	100
1	G	254/263 (97%)	248 (98%)	6 (2%)	0	100	100
1	H	244/263 (93%)	238 (98%)	6 (2%)	0	100	100
All	All	2023/2104 (96%)	1971 (97%)	52 (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	177/186 (95%)	171 (97%)	6 (3%)	32	33
1	B	173/186 (93%)	170 (98%)	3 (2%)	53	60
1	C	167/186 (90%)	165 (99%)	2 (1%)	63	70
1	D	164/186 (88%)	159 (97%)	5 (3%)	36	38
1	E	174/186 (94%)	171 (98%)	3 (2%)	53	60
1	F	169/186 (91%)	167 (99%)	2 (1%)	63	70
1	G	167/186 (90%)	162 (97%)	5 (3%)	36	38
1	H	162/186 (87%)	160 (99%)	2 (1%)	63	70
All	All	1353/1488 (91%)	1325 (98%)	28 (2%)	48	52

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	ILE
1	A	122	LEU

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Mol	Chain	Res	Type
1	A	133[A]	GLU
1	A	133[B]	GLU
1	A	195	LYS
1	A	207	GLN
1	B	111	ILE
1	B	122	LEU
1	B	195	LYS
1	C	111	ILE
1	C	122	LEU
1	D	-4	HIS
1	D	2	GLN
1	D	6	ARG
1	D	43	GLU
1	D	111	ILE
1	E	111	ILE
1	E	122	LEU
1	E	181	ARG
1	F	67	LYS
1	F	111	ILE
1	G	4	GLU
1	G	75	GLU
1	G	111	ILE
1	G	122	LEU
1	G	181	ARG
1	H	111	ILE
1	H	122	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-1	HIS
1	A	207	GLN
1	B	0	HIS
1	B	5	ASN
1	C	56	GLN
1	D	0	HIS
1	D	232	HIS
1	F	0	HIS
1	F	155	GLN
1	H	-3	HIS
1	H	-1	HIS
1	H	5	ASN

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 ⓘ

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	TRS	F	301	-	7,7,7	0.51	0	9,9,9	1.32	1 (11%)
2	TRS	D	301	-	7,7,7	0.56	0	9,9,9	1.00	0
2	TRS	B	301	-	7,7,7	1.10	0	9,9,9	2.15	3 (33%)
2	TRS	G	301	-	7,7,7	1.09	0	9,9,9	3.19	8 (88%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRS	F	301	-	-	9/9/9/9	-
2	TRS	D	301	-	-	9/9/9/9	-
2	TRS	B	301	-	-	6/9/9/9	-
2	TRS	G	301	-	-	3/9/9/9	-

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	TRS	O1-C1-C	-4.94	97.12	110.88
2	B	301	TRS	C2-C-C1	-4.48	98.73	110.66
2	G	301	TRS	C3-C-C2	-3.93	100.18	110.66
2	G	301	TRS	C3-C-C1	3.86	120.94	110.66
2	G	301	TRS	C3-C-N	3.74	117.72	108.17
2	G	301	TRS	C2-C-C1	-2.97	102.75	110.66
2	F	301	TRS	C3-C-N	2.90	115.58	108.17
2	B	301	TRS	C3-C-C2	2.68	117.78	110.66
2	B	301	TRS	C1-C-N	2.14	113.62	108.17
2	G	301	TRS	O3-C3-C	2.08	116.67	110.88
2	G	301	TRS	O2-C2-C	-2.05	105.17	110.88
2	G	301	TRS	C1-C-N	-2.03	103.00	108.17

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	TRS	C1-C-C2-O2
2	B	301	TRS	C3-C-C2-O2
2	B	301	TRS	N-C-C2-O2
2	B	301	TRS	N-C-C3-O3
2	D	301	TRS	C3-C-C2-O2
2	D	301	TRS	C1-C-C3-O3
2	D	301	TRS	N-C-C3-O3
2	F	301	TRS	N-C-C2-O2
2	F	301	TRS	N-C-C3-O3
2	G	301	TRS	N-C-C1-O1
2	D	301	TRS	C3-C-C1-O1
2	D	301	TRS	C1-C-C2-O2
2	F	301	TRS	C2-C-C1-O1
2	F	301	TRS	C1-C-C2-O2
2	F	301	TRS	C1-C-C3-O3
2	G	301	TRS	C2-C-C1-O1
2	B	301	TRS	C1-C-C3-O3
2	D	301	TRS	C2-C-C1-O1
2	D	301	TRS	N-C-C1-O1
2	D	301	TRS	N-C-C2-O2
2	D	301	TRS	C2-C-C3-O3
2	F	301	TRS	N-C-C1-O1
2	G	301	TRS	C3-C-C1-O1

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Mol	Chain	Res	Type	Atoms
2	B	301	TRS	C2-C-C3-O3
2	F	301	TRS	C3-C-C2-O2
2	F	301	TRS	C2-C-C3-O3
2	F	301	TRS	C3-C-C1-O1

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	TRS	1	0
2	B	301	TRS	1	0
2	G	301	TRS	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 [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	260/263 (98%)	-0.93	0 100 100	14, 24, 49, 68	2 (0%)
1	B	260/263 (98%)	-0.77	0 100 100	18, 31, 50, 63	0
1	C	259/263 (98%)	-0.61	0 100 100	21, 35, 61, 67	0
1	D	249/263 (94%)	-0.88	0 100 100	18, 29, 43, 54	0
1	E	257/263 (97%)	-0.93	0 100 100	18, 27, 43, 59	0
1	F	254/263 (96%)	-0.83	0 100 100	21, 30, 48, 63	0
1	G	256/263 (97%)	-0.65	0 100 100	20, 35, 56, 82	0
1	H	248/263 (94%)	-0.85	0 100 100	18, 29, 49, 72	0
All	All	2043/2104 (97%)	-0.80	0 100 100	14, 30, 51, 82	2 (0%)

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
2	TRS	B	301	8/8	0.98	0.05	18,19,20,22	0
2	TRS	D	301	8/8	0.98	0.06	29,37,44,49	0
2	TRS	F	301	8/8	0.98	0.06	23,25,26,29	0
2	TRS	G	301	8/8	0.98	0.05	15,16,19,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.