



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:05 PM UTC

PDB ID : 3D3U / pdb_00003d3u
Title : Crystal structure of 4-hydroxybutyrate CoA-transferase (abfT-2) from Porphyromonas gingivalis. Northeast Structural Genomics Consortium target PgR26
Authors : Forouhar, F.; Neely, H.; Zhang, X.-Z.; Price II, W.N.; Hussain, M.; Seetharaman, J.; Xiao, R.; Conover, K.; Cunningham, K.; Ma, L.-C.; Ho, C.K.; Everett, J.K.; Acton, T.B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2008-05-12
Resolution : 2.80 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
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

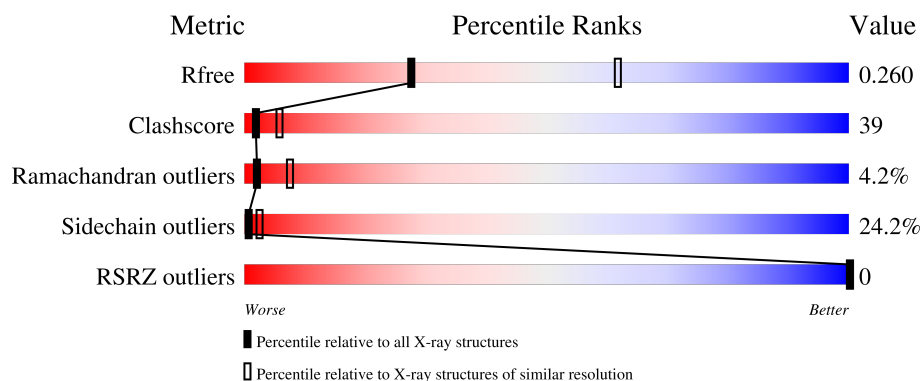
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

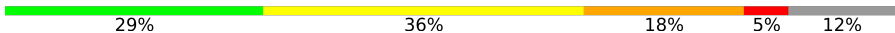
The reported resolution of this entry is 2.80 Å.

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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	439	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3038 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 4-hydroxybutyrate CoA-transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			3018	1909	533	557	19			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	GLY	ILE	expression tag	UNP Q7MTJ6
A	432	LEU	-	expression tag	UNP Q7MTJ6
A	433	GLU	-	expression tag	UNP Q7MTJ6
A	434	HIS	-	expression tag	UNP Q7MTJ6
A	435	HIS	-	expression tag	UNP Q7MTJ6
A	436	HIS	-	expression tag	UNP Q7MTJ6
A	437	HIS	-	expression tag	UNP Q7MTJ6
A	438	HIS	-	expression tag	UNP Q7MTJ6
A	439	HIS	-	expression tag	UNP Q7MTJ6

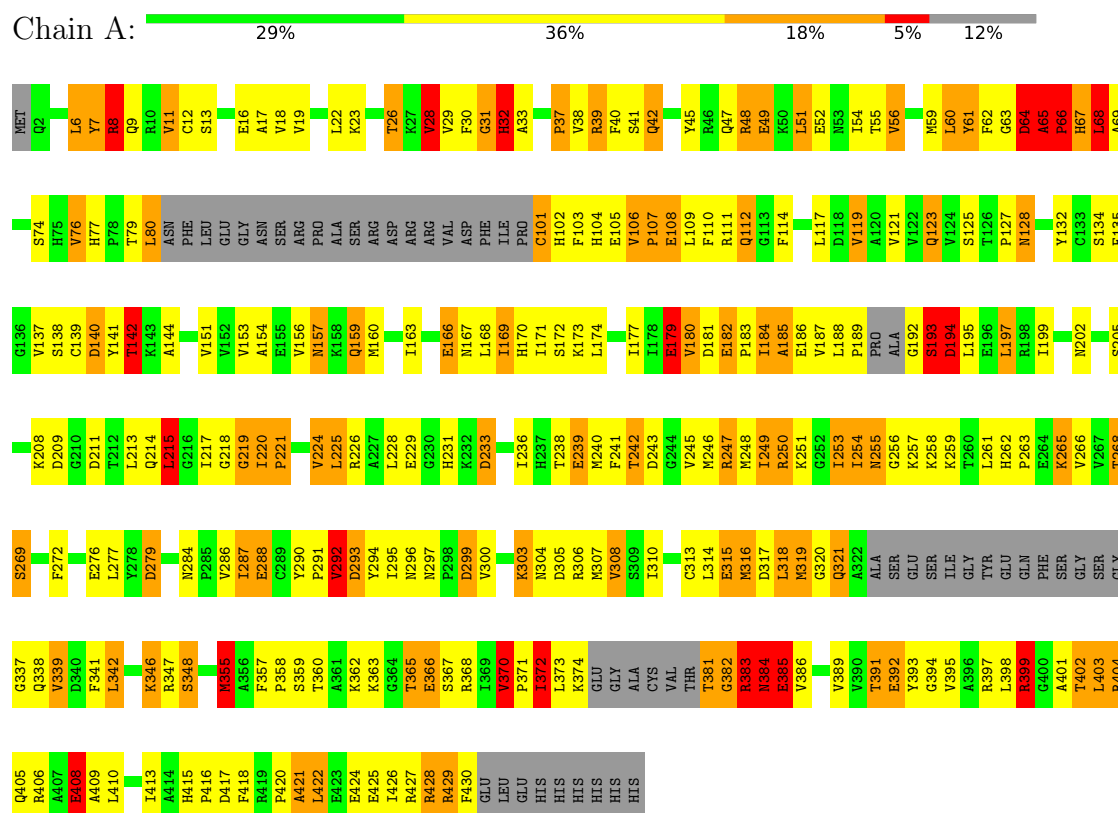
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	20	Total	O	0	0
			20	20		

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: 4-hydroxybutyrate CoA-transferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.68Å 87.28Å 93.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.35 – 2.80 29.35 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.35-2.80) 91.9 (29.35-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.58 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.199 , 0.260 0.200 , 0.260	Depositor DCC
R_{free} test set	505 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3038	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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

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	1.86	46/3076 (1.5%)	1.80	69/4155 (1.7%)

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	ALA	CA-CB	10.86	1.70	1.53
1	A	385	GLU	CA-C	9.86	1.60	1.52
1	A	372	ILE	CA-CB	9.65	1.67	1.54
1	A	63	GLY	N-CA	9.45	1.58	1.45
1	A	383	ARG	N-CA	8.57	1.57	1.46
1	A	123	GLN	C-O	-7.43	1.15	1.23
1	A	144	ALA	CA-CB	-7.39	1.41	1.53
1	A	189	PRO	N-CA	6.95	1.57	1.47
1	A	355	MET	CG-SD	6.82	1.97	1.80
1	A	29	VAL	CA-CB	6.71	1.64	1.54
1	A	184	ILE	C-O	-6.56	1.17	1.24
1	A	370	VAL	CA-CB	-6.56	1.49	1.55
1	A	22	LEU	CA-C	-6.56	1.46	1.53
1	A	67	HIS	C-O	6.54	1.32	1.24
1	A	180	VAL	CA-C	-6.31	1.47	1.52
1	A	268	THR	CA-C	6.31	1.59	1.53
1	A	154	ALA	CA-CB	-6.17	1.44	1.53
1	A	31	GLY	N-CA	6.16	1.53	1.45
1	A	134	SER	CA-C	-6.04	1.45	1.52
1	A	19	VAL	CA-CB	-5.99	1.47	1.54
1	A	346	LYS	CB-CG	5.93	1.70	1.52
1	A	199	ILE	CA-CB	5.87	1.60	1.54
1	A	399	ARG	CG-CD	5.74	1.69	1.52
1	A	239	GLU	N-CA	-5.69	1.38	1.46
1	A	142	THR	N-CA	-5.66	1.39	1.46
1	A	240	MET	C-O	-5.61	1.17	1.23
1	A	262	HIS	C-O	5.59	1.26	1.23
1	A	61	TYR	CB-CG	5.49	1.63	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	ARG	N-CA	5.45	1.52	1.46
1	A	233	ASP	N-CA	5.43	1.53	1.46
1	A	11	VAL	CA-C	5.42	1.58	1.52
1	A	32	HIS	C-O	-5.42	1.16	1.23
1	A	348	SER	CA-C	-5.42	1.45	1.52
1	A	8	ARG	NE-CZ	5.35	1.39	1.33
1	A	194	ASP	CA-C	5.34	1.59	1.52
1	A	321	GLN	N-CA	-5.34	1.40	1.46
1	A	63	GLY	C-O	5.33	1.31	1.24
1	A	28	VAL	CA-C	-5.33	1.46	1.52
1	A	66	PRO	CB-CG	5.29	1.76	1.49
1	A	370	VAL	CA-C	5.20	1.56	1.52
1	A	40	PHE	N-CA	-5.18	1.40	1.46
1	A	157	ASN	N-CA	-5.17	1.39	1.46
1	A	395	VAL	C-O	-5.11	1.18	1.24
1	A	314	LEU	CG-CD2	5.10	1.69	1.52
1	A	240	MET	N-CA	5.05	1.52	1.46
1	A	59	MET	C-O	-5.02	1.17	1.24

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	GLY	CA-C-O	9.31	127.66	119.56
1	A	370	VAL	N-CA-C	8.92	117.74	107.84
1	A	409	ALA	N-CA-C	-8.92	100.99	112.23
1	A	49	GLU	N-CA-C	-8.44	102.42	112.89
1	A	269	SER	N-CA-C	-8.44	103.84	114.56
1	A	224	VAL	CB-CA-C	-8.36	101.07	112.02
1	A	69	ALA	N-CA-C	-8.02	97.72	109.50
1	A	360	THR	N-CA-C	7.95	120.07	108.86
1	A	67	HIS	CB-CA-C	-7.83	94.83	110.42
1	A	249	ILE	N-CA-C	-7.53	103.19	110.42
1	A	211	ASP	CA-C-N	-7.46	113.14	122.84
1	A	211	ASP	C-N-CA	-7.46	113.14	122.84
1	A	383	ARG	N-CA-C	7.35	126.45	110.80
1	A	213	LEU	N-CA-C	7.26	121.22	110.48
1	A	42	GLN	N-CA-C	-7.25	103.31	111.07
1	A	111	ARG	N-CA-C	-7.22	104.91	113.21
1	A	31	GLY	CA-C-N	-7.20	110.14	123.03
1	A	31	GLY	C-N-CA	-7.20	110.14	123.03
1	A	63	GLY	N-CA-C	7.03	122.01	113.79
1	A	404	ARG	N-CA-C	6.93	118.92	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	308	VAL	N-CA-C	6.89	118.24	107.28
1	A	31	GLY	N-CA-C	-6.75	103.90	112.54
1	A	184	ILE	N-CA-CB	-6.70	103.39	110.82
1	A	292	VAL	CB-CA-C	-6.69	101.26	112.16
1	A	68	LEU	N-CA-C	-6.59	105.11	113.02
1	A	180	VAL	N-CA-C	6.49	116.45	108.53
1	A	408	GLU	CB-CA-C	6.30	121.83	109.72
1	A	384	ASN	CA-C-N	6.21	129.72	121.90
1	A	384	ASN	C-N-CA	6.21	129.72	121.90
1	A	7	TYR	N-CA-C	-6.16	103.72	111.11
1	A	279	ASP	N-CA-C	6.15	118.78	111.71
1	A	305	ASP	N-CA-C	6.01	118.97	110.50
1	A	268	THR	N-CA-C	5.95	119.67	108.65
1	A	342	LEU	CA-C-N	5.93	128.15	120.44
1	A	342	LEU	C-N-CA	5.93	128.15	120.44
1	A	382	GLY	CA-C-N	5.87	132.76	121.54
1	A	382	GLY	C-N-CA	5.87	132.76	121.54
1	A	314	LEU	CB-CA-C	5.84	119.91	109.29
1	A	253	ILE	N-CA-C	5.83	116.01	110.53
1	A	101	CYS	CA-CB-SG	-5.81	101.04	114.40
1	A	421	ALA	N-CA-C	-5.78	104.89	111.07
1	A	422	LEU	N-CA-C	5.77	118.31	111.33
1	A	62	PHE	CA-C-O	-5.75	114.64	120.84
1	A	310	ILE	N-CA-C	5.73	116.39	107.28
1	A	52	GLU	CA-C-N	-5.72	114.10	122.06
1	A	52	GLU	C-N-CA	-5.72	114.10	122.06
1	A	413	ILE	N-CA-C	5.71	118.48	112.83
1	A	48	ARG	N-CA-C	5.69	119.03	111.75
1	A	300	VAL	CB-CA-C	-5.65	104.62	112.02
1	A	18	VAL	CA-C-N	-5.65	112.72	120.46
1	A	18	VAL	C-N-CA	-5.65	112.72	120.46
1	A	55	THR	CA-C-N	-5.64	115.83	123.10
1	A	55	THR	C-N-CA	-5.64	115.83	123.10
1	A	17	ALA	N-CA-C	5.50	117.08	111.14
1	A	64	ASP	CA-C-N	-5.48	108.42	121.80
1	A	64	ASP	C-N-CA	-5.48	108.42	121.80
1	A	166	GLU	CB-CA-C	-5.39	104.27	111.88
1	A	32	HIS	N-CA-C	5.39	118.05	109.81
1	A	213	LEU	CB-CA-C	-5.38	99.57	109.46
1	A	128	ASN	N-CA-C	-5.27	101.63	109.96
1	A	139	CYS	N-CA-C	-5.14	104.71	111.96
1	A	179	GLU	N-CA-CB	5.11	117.58	109.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	VAL	CB-CA-C	-5.10	105.17	111.70
1	A	372	ILE	N-CA-C	-5.09	100.20	107.78
1	A	399	ARG	N-CA-CB	5.08	117.61	109.28
1	A	306	ARG	CA-C-N	-5.07	115.46	122.30
1	A	306	ARG	C-N-CA	-5.07	115.46	122.30
1	A	215	LEU	N-CA-C	5.04	117.33	109.52
1	A	288	GLU	N-CA-C	5.01	117.31	108.75

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	3018	0	3019	236	0
2	A	20	0	0	6	0
All	All	3038	0	3019	236	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 39.

All (236) 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:A:66:PRO:CG	1:A:66:PRO:CB	1.76	1.39
1:A:313:CYS:SG	1:A:355:MET:HE2	1.83	1.19
1:A:292:VAL:HA	1:A:295:ILE:HG22	1.38	1.02
1:A:313:CYS:SG	1:A:355:MET:CE	2.53	0.96
1:A:404:ARG:HB3	1:A:430:PHE:CZ	2.01	0.96
1:A:102:HIS:HB2	1:A:105:GLU:OE1	1.65	0.96
1:A:428:ARG:O	1:A:428:ARG:HD3	1.64	0.96
1:A:239:GLU:OE2	1:A:337:GLY:HA3	1.69	0.92
1:A:231:HIS:O	1:A:253:ILE:HD12	1.71	0.91
1:A:428:ARG:O	1:A:429:ARG:HD2	1.77	0.85
1:A:140:ASP:OD1	1:A:142:THR:HG22	1.78	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:PHE:HB2	1:A:167:ASN:OD1	1.81	0.80
1:A:247:ARG:HE	1:A:248:MET:HE2	1.46	0.80
1:A:316:MET:HG3	1:A:317:ASP:N	1.97	0.79
1:A:170:HIS:CD2	1:A:172:SER:H	2.01	0.78
1:A:391:THR:HG22	1:A:393:TYR:H	1.47	0.78
1:A:292:VAL:C	1:A:294:TYR:H	1.91	0.77
1:A:32:HIS:HB3	1:A:141:TYR:OH	1.86	0.76
1:A:313:CYS:HG	1:A:355:MET:CE	1.98	0.76
1:A:256:GLY:CA	1:A:259:LYS:HG3	2.15	0.76
1:A:297:ASN:OD1	1:A:299:ASP:HB2	1.85	0.76
1:A:359:SER:HB3	1:A:391:THR:HG21	1.69	0.75
1:A:415:HIS:CD2	1:A:417:ASP:H	2.04	0.75
1:A:316:MET:HG3	1:A:317:ASP:H	1.52	0.74
1:A:170:HIS:HD2	1:A:172:SER:H	1.36	0.74
1:A:266:VAL:CG2	1:A:287:ILE:HG13	2.17	0.73
1:A:103:PHE:O	1:A:106:VAL:HG23	1.89	0.73
1:A:429:ARG:O	1:A:430:PHE:CD2	2.42	0.72
1:A:358:PRO:O	1:A:368:ARG:HD2	1.92	0.69
1:A:269:SER:HB2	1:A:295:ILE:HG21	1.76	0.67
1:A:242:THR:HG23	1:A:272:PHE:O	1.94	0.67
1:A:248:MET:HB2	1:A:254:ILE:HD12	1.76	0.66
1:A:321:GLN:O	1:A:373:LEU:HD21	1.95	0.66
1:A:128:ASN:C	1:A:128:ASN:OD1	2.38	0.66
1:A:169:ILE:HD11	1:A:173:LYS:HB2	1.76	0.66
1:A:428:ARG:O	1:A:429:ARG:CD	2.43	0.65
1:A:224:VAL:HG12	1:A:228:LEU:HD11	1.78	0.64
1:A:242:THR:HG22	1:A:243:ASP:H	1.61	0.64
1:A:292:VAL:C	1:A:294:TYR:N	2.55	0.64
1:A:246:MET:HE1	1:A:276:GLU:HG2	1.80	0.63
1:A:30:PHE:HE1	1:A:67:HIS:CE1	2.16	0.63
1:A:74:SER:H	1:A:77:HIS:HE1	1.45	0.62
1:A:68:LEU:HB2	2:A:455:HOH:O	1.99	0.62
1:A:415:HIS:HD2	1:A:417:ASP:H	1.45	0.62
1:A:304:ASN:O	1:A:348:SER:HB2	1.99	0.62
1:A:74:SER:H	1:A:77:HIS:CE1	2.17	0.61
1:A:304:ASN:CB	1:A:307:MET:HE2	2.30	0.61
1:A:313:CYS:SG	1:A:355:MET:SD	2.93	0.61
1:A:371:PRO:HB3	1:A:425:GLU:HG2	1.83	0.61
1:A:67:HIS:HB2	2:A:455:HOH:O	2.01	0.61
1:A:51:LEU:HD22	1:A:51:LEU:H	1.65	0.61
1:A:304:ASN:HB3	1:A:307:MET:HE2	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:MET:CB	1:A:254:ILE:HD12	2.32	0.60
1:A:362:LYS:O	1:A:365:THR:OG1	2.20	0.60
1:A:106:VAL:HB	1:A:107:PRO:HD3	1.83	0.59
1:A:238:THR:O	1:A:268:THR:HG22	2.02	0.59
1:A:321:GLN:HE21	1:A:383:ARG:H	1.51	0.59
1:A:383:ARG:HB2	1:A:406:ARG:HH21	1.68	0.59
1:A:60:LEU:CD2	1:A:60:LEU:N	2.65	0.59
1:A:107:PRO:HG2	1:A:292:VAL:HG23	1.85	0.59
1:A:9:GLN:O	1:A:9:GLN:HG2	2.02	0.58
1:A:110:PHE:C	1:A:112:GLN:H	2.11	0.58
1:A:316:MET:CG	1:A:317:ASP:N	2.66	0.58
1:A:159:GLN:NE2	1:A:181:ASP:OD1	2.36	0.57
1:A:238:THR:OG1	1:A:268:THR:CG2	2.52	0.57
1:A:255:ASN:ND2	1:A:257:LYS:HG3	2.20	0.57
1:A:202:ASN:ND2	1:A:394:GLY:HA2	2.19	0.57
1:A:317:ASP:HA	1:A:370:VAL:O	2.05	0.56
1:A:241:PHE:HB2	1:A:245:VAL:HG21	1.87	0.56
1:A:256:GLY:HA2	1:A:259:LYS:HG3	1.85	0.56
1:A:292:VAL:HA	1:A:295:ILE:CG2	2.24	0.56
1:A:123:GLN:NE2	1:A:157:ASN:HD22	2.03	0.56
1:A:359:SER:HB3	1:A:391:THR:CG2	2.35	0.56
1:A:160:MET:HE2	1:A:184:ILE:CD1	2.35	0.56
1:A:104:HIS:HB3	1:A:296:ASN:CB	2.36	0.55
1:A:31:GLY:HA2	1:A:142:THR:HB	1.89	0.55
1:A:104:HIS:HB3	1:A:296:ASN:HB3	1.88	0.55
1:A:163:ILE:HG23	1:A:287:ILE:HG22	1.89	0.55
1:A:317:ASP:HB3	1:A:373:LEU:HG	1.87	0.55
1:A:220:ILE:O	1:A:224:VAL:HG23	2.07	0.55
1:A:408:GLU:HB3	1:A:426:ILE:HD13	1.88	0.55
1:A:214:GLN:HA	1:A:238:THR:HG22	1.88	0.55
1:A:367:SER:HB2	1:A:418:PHE:CD1	2.42	0.55
1:A:224:VAL:HG12	1:A:228:LEU:CD1	2.36	0.54
1:A:48:ARG:HA	1:A:51:LEU:HD23	1.89	0.54
1:A:397:ARG:HB2	1:A:397:ARG:CZ	2.36	0.54
1:A:121:VAL:HG22	1:A:153:VAL:HB	1.90	0.54
1:A:106:VAL:O	1:A:107:PRO:C	2.50	0.54
1:A:246:MET:CE	1:A:276:GLU:HG2	2.38	0.54
1:A:102:HIS:HD2	1:A:339:VAL:HG11	1.72	0.53
1:A:184:ILE:O	1:A:185:ALA:C	2.50	0.53
1:A:256:GLY:HA3	1:A:259:LYS:HG3	1.88	0.53
1:A:159:GLN:HG2	1:A:183:PRO:HA	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:GLN:HG2	1:A:238:THR:HG22	1.91	0.53
1:A:401:ALA:O	1:A:406:ARG:HD2	2.09	0.53
1:A:266:VAL:HG23	1:A:266:VAL:O	2.09	0.52
1:A:238:THR:OG1	1:A:268:THR:HG22	2.09	0.52
1:A:266:VAL:HG23	1:A:287:ILE:HG13	1.92	0.52
1:A:194:ASP:CG	1:A:195:LEU:H	2.18	0.52
1:A:13:SER:OG	1:A:16:GLU:HG3	2.09	0.52
1:A:428:ARG:O	1:A:428:ARG:CD	2.49	0.52
1:A:255:ASN:HD22	1:A:257:LYS:H	1.58	0.52
1:A:41:SER:OG	1:A:67:HIS:CE1	2.63	0.52
1:A:225:LEU:HB3	1:A:248:MET:HE3	1.91	0.52
1:A:258:LYS:O	1:A:259:LYS:C	2.52	0.52
1:A:261:LEU:HD22	1:A:303:LYS:HB2	1.92	0.51
1:A:318:LEU:HD21	1:A:422:LEU:HD22	1.92	0.51
1:A:286:VAL:O	1:A:286:VAL:HG22	2.09	0.51
1:A:123:GLN:HE21	1:A:157:ASN:HD22	1.59	0.51
1:A:402:THR:HB	1:A:404:ARG:HD3	1.92	0.51
1:A:160:MET:CE	1:A:184:ILE:HD12	2.41	0.51
1:A:342:LEU:HD21	1:A:386:VAL:HG22	1.93	0.51
1:A:60:LEU:N	1:A:60:LEU:HD23	2.25	0.50
1:A:315:GLU:HG2	1:A:373:LEU:HD23	1.93	0.50
1:A:160:MET:HE2	1:A:184:ILE:HD11	1.92	0.50
1:A:383:ARG:C	1:A:385:GLU:H	2.19	0.50
1:A:402:THR:O	1:A:403:LEU:C	2.55	0.50
1:A:304:ASN:O	1:A:348:SER:CB	2.59	0.50
1:A:402:THR:OG1	1:A:405:GLN:HG3	2.11	0.50
1:A:23:LYS:O	1:A:26:THR:OG1	2.29	0.49
1:A:246:MET:O	1:A:250:ARG:HB2	2.12	0.49
1:A:236:ILE:HB	1:A:266:VAL:HG12	1.94	0.49
1:A:220:ILE:HB	1:A:221:PRO:HD3	1.93	0.49
1:A:51:LEU:HD22	1:A:51:LEU:N	2.27	0.49
1:A:290:TYR:HB3	1:A:291:PRO:HD2	1.94	0.49
1:A:229:GLU:OE1	1:A:251:LYS:HE2	2.13	0.49
1:A:61:TYR:CG	1:A:61:TYR:O	2.66	0.48
1:A:245:VAL:O	1:A:249:ILE:HG13	2.12	0.48
1:A:28:VAL:HG22	1:A:56:VAL:HB	1.95	0.48
1:A:54:ILE:HB	1:A:76:VAL:HB	1.95	0.48
1:A:215:LEU:H	1:A:238:THR:HG22	1.78	0.48
1:A:398:LEU:O	1:A:399:ARG:C	2.56	0.48
1:A:391:THR:HG22	1:A:393:TYR:N	2.22	0.48
1:A:265:LYS:HB3	1:A:265:LYS:NZ	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:GLU:HB3	1:A:426:ILE:CD1	2.43	0.48
1:A:68:LEU:N	2:A:455:HOH:O	2.46	0.48
1:A:193:SER:O	1:A:197:LEU:HB2	2.14	0.47
1:A:317:ASP:C	1:A:319:MET:H	2.22	0.47
1:A:403:LEU:HA	1:A:403:LEU:HD23	1.58	0.47
1:A:401:ALA:HB3	1:A:406:ARG:CG	2.45	0.47
1:A:415:HIS:CG	1:A:416:PRO:HD2	2.48	0.47
1:A:169:ILE:HD12	1:A:174:LEU:CD1	2.45	0.47
1:A:215:LEU:HD12	1:A:221:PRO:HB3	1.96	0.47
1:A:363:LYS:O	1:A:363:LYS:HG2	2.14	0.47
1:A:226:ARG:O	1:A:229:GLU:HG3	2.14	0.47
1:A:365:THR:C	1:A:366:GLU:HG2	2.38	0.47
1:A:160:MET:CE	1:A:184:ILE:CD1	2.92	0.47
1:A:397:ARG:CZ	1:A:397:ARG:CB	2.93	0.47
1:A:119:VAL:HA	1:A:151:VAL:O	2.14	0.46
1:A:171:ILE:HD12	1:A:174:LEU:HD22	1.97	0.46
1:A:304:ASN:HB2	1:A:307:MET:HE2	1.97	0.46
1:A:381:THR:O	1:A:381:THR:OG1	2.27	0.46
1:A:391:THR:O	1:A:392:GLU:C	2.56	0.46
1:A:103:PHE:CD2	1:A:106:VAL:HG21	2.51	0.46
1:A:197:LEU:HD12	1:A:197:LEU:HA	1.75	0.46
1:A:236:ILE:O	1:A:259:LYS:NZ	2.48	0.46
1:A:215:LEU:CD1	1:A:221:PRO:HB3	2.46	0.46
1:A:421:ALA:O	1:A:424:GLU:HB3	2.16	0.45
1:A:321:GLN:NE2	1:A:382:GLY:HA2	2.31	0.45
1:A:255:ASN:HD22	1:A:255:ASN:C	2.25	0.45
1:A:265:LYS:HD3	1:A:288:GLU:OE1	2.17	0.45
1:A:404:ARG:HB3	1:A:430:PHE:HZ	1.72	0.45
1:A:242:THR:HG22	1:A:243:ASP:OD2	2.17	0.45
1:A:259:LYS:HB2	1:A:263:PRO:HA	1.99	0.45
1:A:8:ARG:NH2	1:A:179:GLU:OE1	2.49	0.45
1:A:65:ALA:HA	2:A:454:HOH:O	2.16	0.45
1:A:218:GLY:O	1:A:219:GLY:C	2.57	0.44
1:A:45:TYR:HB2	1:A:66:PRO:CB	2.47	0.44
1:A:102:HIS:HD2	1:A:339:VAL:CG1	2.30	0.44
1:A:208:LYS:O	1:A:209:ASP:C	2.55	0.44
1:A:181:ASP:OD1	1:A:181:ASP:C	2.59	0.44
1:A:242:THR:CG2	1:A:243:ASP:H	2.25	0.44
1:A:342:LEU:HD23	1:A:385:GLU:HG3	1.99	0.44
1:A:383:ARG:HD3	1:A:384:ASN:H	1.83	0.44
1:A:401:ALA:CB	1:A:406:ARG:HG3	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:ASP:O	1:A:420:PRO:HD2	2.17	0.44
1:A:316:MET:HE1	1:A:389:VAL:HG21	1.99	0.44
1:A:408:GLU:CB	1:A:426:ILE:CD1	2.96	0.44
1:A:140:ASP:O	1:A:292:VAL:HG22	2.17	0.44
1:A:316:MET:HE3	1:A:320:GLY:HA2	1.99	0.43
1:A:383:ARG:HD3	1:A:384:ASN:ND2	2.33	0.43
1:A:214:GLN:HG3	1:A:341:PHE:CZ	2.53	0.43
1:A:287:ILE:C	1:A:288:GLU:HG3	2.42	0.43
1:A:357:PHE:HB2	1:A:358:PRO:CD	2.48	0.43
1:A:391:THR:CG2	1:A:392:GLU:N	2.80	0.43
1:A:156:VAL:CG2	1:A:177:ILE:HG23	2.49	0.43
1:A:6:LEU:HA	1:A:6:LEU:HD12	1.67	0.43
1:A:108:GLU:O	1:A:112:GLN:HB3	2.19	0.43
1:A:192:GLY:O	1:A:193:SER:HB3	2.18	0.43
1:A:255:ASN:ND2	1:A:257:LYS:H	2.16	0.43
1:A:255:ASN:CG	1:A:257:LYS:HG3	2.44	0.43
1:A:140:ASP:C	1:A:292:VAL:HG22	2.43	0.43
1:A:268:THR:HB	1:A:269:SER:H	1.45	0.43
1:A:110:PHE:O	1:A:112:GLN:N	2.52	0.42
1:A:8:ARG:HA	1:A:8:ARG:HD3	1.77	0.42
1:A:65:ALA:N	1:A:66:PRO:HD2	2.34	0.42
1:A:179:GLU:O	1:A:180:VAL:HG13	2.19	0.42
1:A:209:ASP:OD1	1:A:209:ASP:N	2.53	0.42
1:A:319:MET:HE2	1:A:319:MET:HB2	1.82	0.42
1:A:233:ASP:HA	1:A:255:ASN:HD21	1.85	0.42
1:A:140:ASP:OD1	1:A:141:TYR:N	2.48	0.42
1:A:420:PRO:O	1:A:424:GLU:HB2	2.19	0.42
1:A:265:LYS:HD3	1:A:288:GLU:CD	2.45	0.42
1:A:39:ARG:NH2	1:A:182:GLU:OE1	2.53	0.42
1:A:47:GLN:O	1:A:51:LEU:HD22	2.19	0.42
1:A:101:CYS:SG	1:A:102:HIS:N	2.92	0.42
1:A:171:ILE:HD12	1:A:171:ILE:HA	1.86	0.42
1:A:284:ASN:OD1	1:A:284:ASN:C	2.63	0.42
1:A:48:ARG:HA	1:A:51:LEU:CD2	2.48	0.42
1:A:259:LYS:HE3	1:A:259:LYS:HB3	1.76	0.42
1:A:371:PRO:HG2	1:A:372:ILE:HG22	2.02	0.42
1:A:37:PRO:HG2	1:A:121:VAL:HG12	2.02	0.41
1:A:61:TYR:HB2	1:A:64:ASP:OD1	2.20	0.41
1:A:215:LEU:H	1:A:238:THR:CG2	2.33	0.41
1:A:292:VAL:O	1:A:294:TYR:N	2.53	0.41
1:A:112:GLN:HG2	1:A:114:PHE:CE1	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ALA:HB2	2:A:454:HOH:O	2.20	0.41
1:A:80:LEU:H	1:A:80:LEU:HD13	1.85	0.41
1:A:297:ASN:OD1	1:A:299:ASP:CB	2.62	0.41
1:A:127:PRO:HA	1:A:132:TYR:O	2.20	0.41
1:A:372:ILE:HD12	1:A:373:LEU:O	2.21	0.41
1:A:226:ARG:HD3	1:A:226:ARG:HA	1.99	0.41
1:A:65:ALA:HB3	1:A:66:PRO:CD	2.50	0.41
1:A:391:THR:C	1:A:393:TYR:N	2.79	0.41
1:A:12:CYS:HB2	1:A:16:GLU:OE1	2.21	0.41
1:A:32:HIS:HD2	1:A:60:LEU:H	1.68	0.41
1:A:107:PRO:HB2	1:A:293:ASP:HB3	2.02	0.41
1:A:125:SER:HA	1:A:160:MET:HB3	2.02	0.41
1:A:233:ASP:HA	1:A:255:ASN:ND2	2.36	0.41
1:A:269:SER:HA	1:A:290:TYR:O	2.21	0.41
1:A:391:THR:HG22	1:A:392:GLU:N	2.36	0.41
1:A:6:LEU:O	1:A:7:TYR:C	2.64	0.40
1:A:363:LYS:O	1:A:363:LYS:CG	2.69	0.40
1:A:241:PHE:CD2	1:A:241:PHE:C	2.99	0.40
1:A:362:LYS:HD3	1:A:365:THR:OG1	2.21	0.40
1:A:186:GLU:HG2	2:A:453:HOH:O	2.22	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	377/439 (86%)	327 (87%)	34 (9%)	16 (4%)	2 7

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	66	PRO
1	A	140	ASP
1	A	193	SER
1	A	194	ASP
1	A	384	ASN
1	A	429	ARG
1	A	33	ALA
1	A	318	LEU
1	A	392	GLU
1	A	185	ALA
1	A	403	LEU
1	A	65	ALA
1	A	219	GLY
1	A	293	ASP
1	A	37	PRO

5.3.2 Protein sidechains [i](#)

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	327/370 (88%)	248 (76%)	79 (24%)	1 2

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	8	ARG
1	A	11	VAL
1	A	26	THR
1	A	28	VAL
1	A	32	HIS
1	A	38	VAL
1	A	42	GLN
1	A	49	GLU
1	A	51	LEU
1	A	56	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	60	LEU
1	A	68	LEU
1	A	76	VAL
1	A	79	THR
1	A	80	LEU
1	A	106	VAL
1	A	107	PRO
1	A	108	GLU
1	A	109	LEU
1	A	112	GLN
1	A	117	LEU
1	A	119	VAL
1	A	137	VAL
1	A	138	SER
1	A	142	THR
1	A	159	GLN
1	A	166	GLU
1	A	168	LEU
1	A	169	ILE
1	A	179	GLU
1	A	182	GLU
1	A	187	VAL
1	A	188	LEU
1	A	193	SER
1	A	197	LEU
1	A	205	SER
1	A	215	LEU
1	A	217	ILE
1	A	220	ILE
1	A	221	PRO
1	A	225	LEU
1	A	242	THR
1	A	247	ARG
1	A	250	ARG
1	A	254	ILE
1	A	255	ASN
1	A	265	LYS
1	A	277	LEU
1	A	279	ASP
1	A	287	ILE
1	A	292	VAL
1	A	299	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	303	LYS
1	A	308	VAL
1	A	315	GLU
1	A	316	MET
1	A	319	MET
1	A	338	GLN
1	A	339	VAL
1	A	346	LYS
1	A	347	ARG
1	A	355	MET
1	A	365	THR
1	A	366	GLU
1	A	370	VAL
1	A	372	ILE
1	A	374	LYS
1	A	381	THR
1	A	383	ARG
1	A	384	ASN
1	A	385	GLU
1	A	391	THR
1	A	399	ARG
1	A	402	THR
1	A	408	GLU
1	A	410	LEU
1	A	427	ARG
1	A	428	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	9	GLN
1	A	32	HIS
1	A	58	HIS
1	A	67	HIS
1	A	77	HIS
1	A	102	HIS
1	A	104	HIS
1	A	112	GLN
1	A	123	GLN
1	A	170	HIS
1	A	202	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	214	GLN
1	A	231	HIS
1	A	255	ASN
1	A	321	GLN
1	A	338	GLN
1	A	384	ASN
1	A	415	HIS

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	387/439 (88%)	-0.37	0 100 100	5, 23, 38, 47	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.