



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:02 AM GMT

PDB ID : 3D3U
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

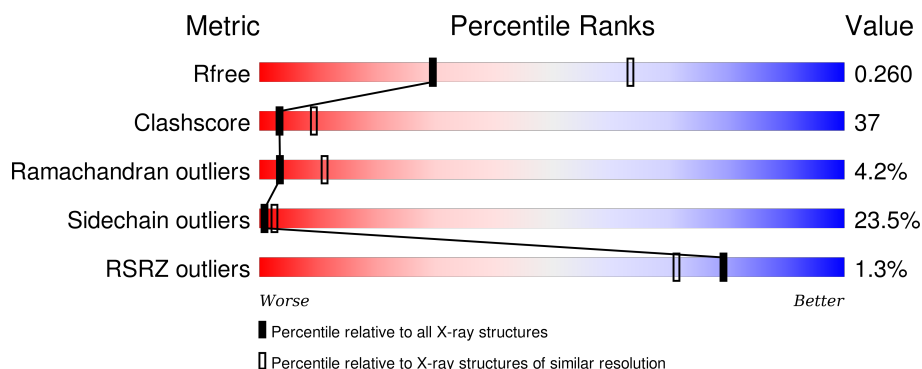
1 Overall quality at a glance

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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div></div> <div> <div></div> <div>34%</div> <div>35%</div> <div>15%</div> <div>•</div> <div>12%</div> </div> </div>

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

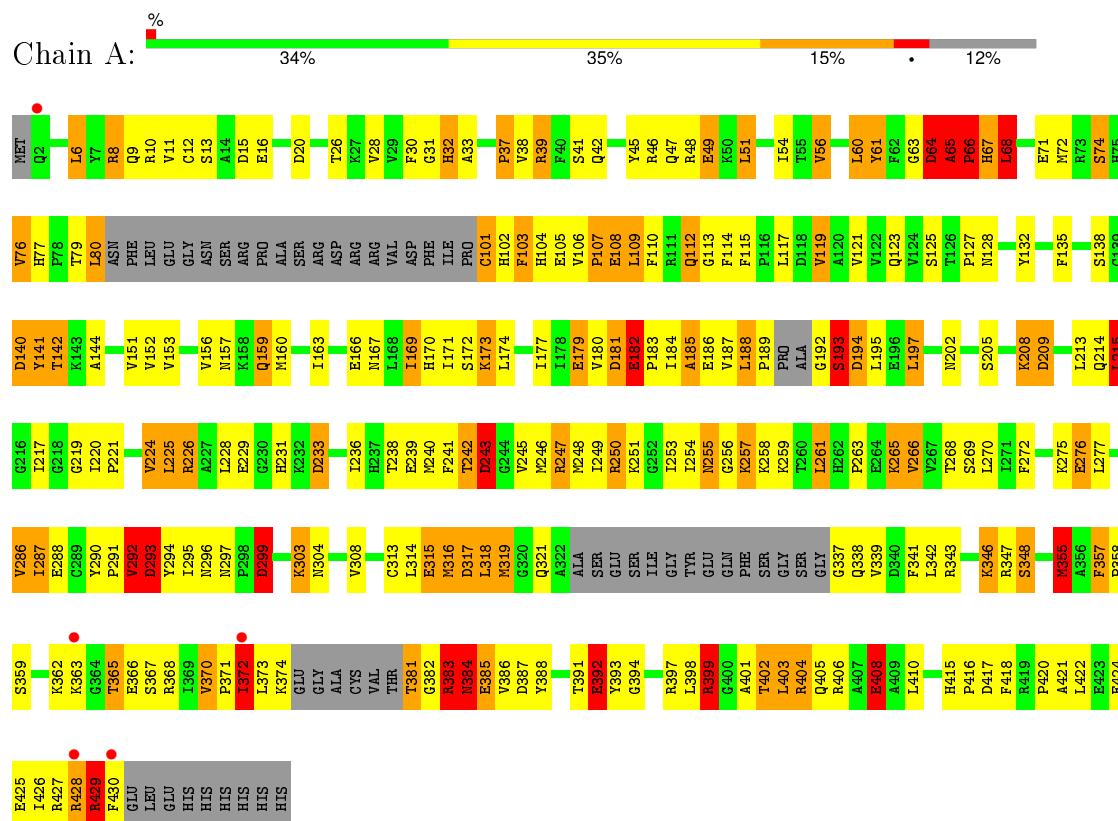
- Molecule 2 is water.

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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 27.56 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.35-2.80) 92.0 (27.56-2.80)	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 (5.01%)	DCC
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 59.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 10594 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.55	32/3076 (1.0%)	1.45	42/4155 (1.0%)

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	TYR	CD1-CE1	9.22	1.53	1.39
1	A	65	ALA	CA-CB	8.64	1.70	1.52
1	A	63	GLY	N-CA	8.26	1.58	1.46
1	A	61	TYR	CB-CG	8.06	1.63	1.51
1	A	392	GLU	CD-OE1	8.03	1.34	1.25
1	A	61	TYR	CD2-CE2	7.79	1.51	1.39
1	A	61	TYR	CG-CD2	7.19	1.48	1.39
1	A	399	ARG	CG-CD	7.09	1.69	1.51
1	A	357	PHE	CE2-CZ	7.08	1.50	1.37
1	A	115	PHE	CE1-CZ	6.73	1.50	1.37
1	A	346	LYS	CB-CG	6.55	1.70	1.52
1	A	11	VAL	CB-CG1	-6.51	1.39	1.52
1	A	355	MET	CG-SD	6.40	1.97	1.81
1	A	182	GLU	CG-CD	6.39	1.61	1.51
1	A	61	TYR	CG-CD1	6.35	1.47	1.39
1	A	182	GLU	CD-OE1	6.26	1.32	1.25
1	A	141	TYR	CE2-CZ	-6.09	1.30	1.38
1	A	189	PRO	N-CA	6.02	1.57	1.47
1	A	173	LYS	CE-NZ	5.90	1.63	1.49
1	A	49	GLU	CG-CD	5.75	1.60	1.51
1	A	64	ASP	CB-CG	-5.53	1.40	1.51
1	A	71	GLU	CD-OE1	-5.50	1.19	1.25
1	A	113	GLY	N-CA	-5.48	1.37	1.46
1	A	383	ARG	N-CA	5.45	1.57	1.46
1	A	266	VAL	CB-CG2	-5.29	1.41	1.52
1	A	372	ILE	CA-CB	5.26	1.67	1.54
1	A	66	PRO	CB-CG	5.23	1.76	1.50
1	A	286	VAL	CB-CG2	-5.16	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	388	TYR	CB-CG	-5.16	1.44	1.51
1	A	152	VAL	CB-CG2	-5.14	1.42	1.52
1	A	115	PHE	CG-CD2	5.09	1.46	1.38
1	A	144	ALA	CA-CB	-5.09	1.41	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	ASP	CB-CG-OD2	9.15	126.53	118.30
1	A	20	ASP	CB-CG-OD2	8.73	126.16	118.30
1	A	6	LEU	CB-CG-CD1	-7.88	97.61	111.00
1	A	67	HIS	CB-CA-C	-7.79	94.83	110.40
1	A	226	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	A	15	ASP	CB-CG-OD2	7.42	124.97	118.30
1	A	101	CYS	CA-CB-SG	-7.20	101.04	114.00
1	A	225	LEU	CB-CG-CD2	-7.15	98.84	111.00
1	A	181	ASP	CB-CG-OD2	7.14	124.72	118.30
1	A	209	ASP	CB-CG-OD2	6.81	124.43	118.30
1	A	343	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	A	46	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	A	355	MET	CG-SD-CE	6.74	110.99	100.20
1	A	71	GLU	OE1-CD-OE2	-6.65	115.32	123.30
1	A	109	LEU	CB-CG-CD2	-6.51	99.94	111.00
1	A	314	LEU	CB-CG-CD2	6.40	121.88	111.00
1	A	188	LEU	CA-CB-CG	6.24	129.64	115.30
1	A	233	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	317	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	243	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	399	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	10	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	383	ARG	N-CA-C	5.72	126.45	111.00
1	A	408	GLU	CB-CA-C	5.71	121.83	110.40
1	A	387	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	299	ASP	CB-CG-OD1	-5.66	113.21	118.30
1	A	208	LYS	CD-CE-NZ	5.64	124.67	111.70
1	A	213	LEU	CB-CA-C	-5.60	99.57	110.20
1	A	293	ASP	CB-CG-OD1	-5.53	113.33	118.30
1	A	226	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	275	LYS	CD-CE-NZ	-5.47	99.11	111.70
1	A	224	VAL	CB-CA-C	-5.44	101.07	111.40
1	A	10	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	72	MET	CG-SD-CE	5.41	108.85	100.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	LEU	CA-CB-CG	5.34	127.59	115.30
1	A	292	VAL	CB-CA-C	-5.34	101.26	111.40
1	A	64	ASP	C-N-CA	-5.31	108.42	121.70
1	A	68	LEU	CB-CG-CD1	5.28	119.97	111.00
1	A	261	LEU	CB-CG-CD1	-5.20	102.16	111.00
1	A	240	MET	CG-SD-CE	5.19	108.50	100.20
1	A	314	LEU	CB-CA-C	5.11	119.91	110.20
1	A	64	ASP	CB-CG-OD2	-5.10	113.71	118.30

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	221	0
2	A	20	0	0	6	0
All	All	3038	0	3019	221	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 37.

All (221) 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:CB	1:A:66:PRO:CG	1.76	1.39
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	0.97
1:A:404:ARG:HB3	1:A:430:PHE:CZ	2.01	0.96
1:A:428:ARG:HD3	1:A:428:ARG:O	1.64	0.96
1:A:102:HIS:HB2	1:A:105:GLU:OE1	1.65	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: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: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:313:CYS:SG	1:A:355:MET:HE2	2.28	0.73
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:292:VAL:C	1:A:294:TYR:H	1.91	0.72
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:313:CYS:SG	1:A:355:MET:HE1	2.33	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: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: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: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:128:ASN:OD1	1:A:128:ASN:C	2.38	0.61
1:A:51:LEU:H	1:A:51:LEU:HD22	1.65	0.61
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:THR:O	1:A:268:THR:HG22	2.02	0.59
1:A:292:VAL:C	1:A:294:TYR:N	2.55	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:N	1:A:60:LEU:CD2	2.65	0.59
1:A:107:PRO:HG2	1:A:292:VAL:HG23	1.85	0.59
1:A:9:GLN:HG2	1:A:9:GLN:O	2.02	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:292:VAL:HA	1:A:295:ILE:CG2	2.24	0.56
1:A:256:GLY:HA2	1:A:259:LYS:HG3	1.85	0.56
1:A:241:PHE:HB2	1:A:245:VAL:HG21	1.87	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: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:317:ASP:HB3	1:A:373:LEU:HG	1.87	0.55
1:A:163:ILE:HG23	1:A:287:ILE:HG22	1.89	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:CZ	1:A:397:ARG:HB2	2.36	0.54
1:A:121:VAL:HG22	1:A:153:VAL:HB	1.90	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:110:PHE:C	1:A:112:GLN:H	2.11	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
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:O	1:A:266:VAL:HG23	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ARG:CD	1:A:428:ARG:O	2.49	0.52
1:A:13:SER:OG	1:A:16:GLU:HG3	2.09	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: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: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: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:106:VAL:O	1:A:107:PRO:C	2.50	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:184:ILE:O	1:A:185:ALA:C	2.50	0.49
1:A:229:GLU:OE1	1:A:251:LYS:HE2	2.13	0.49
1:A:245:VAL:O	1:A:249:ILE:HG13	2.12	0.48
1:A:61:TYR:CG	1:A:61:TYR:O	2.66	0.48
1:A:215:LEU:H	1:A:238:THR:HG22	1.78	0.48
1:A:54:ILE:HB	1:A:76:VAL:HB	1.95	0.48
1:A:28:VAL:HG22	1:A:56:VAL:HB	1.95	0.48
1:A:391:THR:HG22	1:A:393:TYR:N	2.22	0.48
1:A:265:LYS:NZ	1:A:265:LYS:HB3	2.28	0.48
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:403:LEU:HD23	1:A:403:LEU:HA	1.58	0.47
1:A:194:ASP:CG	1:A:195:LEU:H	2.18	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:258:LYS:O	1:A:259:LYS:C	2.52	0.47
1:A:363:LYS:O	1:A:363:LYS:HG2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ARG:O	1:A:229:GLU:HG3	2.14	0.47
1:A:397:ARG:CZ	1:A:397:ARG:CB	2.93	0.47
1:A:160:MET:CE	1:A:184:ILE:CD1	2.92	0.47
1:A:171:ILE:HD12	1:A:174:LEU:HD22	1.97	0.46
1:A:119:VAL:HA	1:A:151:VAL:O	2.14	0.46
1:A:381:THR:O	1:A:381:THR:OG1	2.27	0.46
1:A:247:ARG:HE	1:A:248:MET:CE	2.28	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:402:THR:O	1:A:403:LEU:C	2.55	0.46
1:A:383:ARG:C	1:A:385:GLU:H	2.19	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:247:ARG:HE	1:A:248:MET:HE1	1.82	0.45
1:A:404:ARG:HB3	1:A:430:PHE:HZ	1.72	0.45
1:A:265:LYS:HD3	1:A:288:GLU:OE1	2.17	0.45
1:A:259:LYS:HB2	1:A:263:PRO:HA	1.99	0.45
1:A:242:THR:HG22	1:A:243:ASP:OD2	2.17	0.45
1:A:65:ALA:HA	2:A:454:HOH:O	2.16	0.45
1:A:8:ARG:NH2	1:A:179:GLU:OE1	2.49	0.45
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:342:LEU:HD23	1:A:385:GLU:HG3	1.99	0.44
1:A:242:THR:CG2	1:A:243:ASP:H	2.25	0.44
1:A:246:MET:HE1	1:A:276:GLU:HG2	2.00	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
1:A:417:ASP:O	1:A:420:PRO:HD2	2.17	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:398:LEU:O	1:A:399:ARG:C	2.56	0.44
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:160:MET:HE1	1:A:184:ILE:HD12	2.00	0.43
1:A:391:THR:CG2	1:A:392:GLU:N	2.80	0.43
1:A:357:PHE:HB2	1:A:358:PRO:CD	2.48	0.43
1:A:156:VAL:CG2	1:A:177:ILE:HG23	2.49	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LEU:HA	1:A:6:LEU:HD12	1.67	0.43
1:A:255:ASN:ND2	1:A:257:LYS:H	2.16	0.43
1:A:317:ASP:C	1:A:319:MET:H	2.22	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: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:8:ARG:HD3	1:A:8:ARG:HA	1.77	0.42
1:A:209:ASP:N	1:A:209:ASP:OD1	2.53	0.42
1:A:110:PHE:C	1:A:112:GLN:N	2.72	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:101:CYS:SG	1:A:102:HIS:N	2.92	0.42
1:A:171:ILE:HA	1:A:171:ILE:HD12	1.86	0.42
1:A:47:GLN:O	1:A:51:LEU:HD22	2.19	0.42
1:A:39:ARG:NH2	1:A:182:GLU:OE1	2.53	0.42
1:A:371:PRO:HG2	1:A:372:ILE:HG22	2.02	0.42
1:A:259:LYS:HB3	1:A:259:LYS:HE3	1.76	0.42
1:A:48:ARG:HA	1:A:51:LEU:CD2	2.48	0.42
1:A:160:MET:HE2	1:A:184:ILE:CD1	2.49	0.42
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: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:391:THR:O	1:A:392:GLU:C	2.56	0.41
1:A:112:GLN:HG2	1:A:114:PHE:CE1	2.56	0.41
1:A:65:ALA:HB2	2:A:454:HOH:O	2.20	0.41
1:A:297:ASN:OD1	1:A:299:ASP:CB	2.62	0.41
1:A:80:LEU:HD13	1:A:80:LEU:H	1.85	0.41
1:A:372:ILE:HD12	1:A:373:LEU:O	2.21	0.41
1:A:127:PRO:HA	1:A:132:TYR:O	2.20	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:269:SER:HA	1:A:290:TYR:O	2.21	0.41
1:A:107:PRO:HB2	1:A:293:ASP:HB3	2.02	0.41
1:A:32:HIS:HD2	1:A:60:LEU:H	1.68	0.41
1:A:391:THR:HG22	1:A:392:GLU:N	2.36	0.41
1:A:233:ASP:HA	1:A:255:ASN:ND2	2.36	0.41
1:A:12:CYS:HB2	1:A:16:GLU:OE1	2.21	0.41
1:A:125:SER:HA	1:A:160:MET:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ASN:C	1:A:255:ASN:HD22	2.25	0.40
1:A:363:LYS:O	1:A:363:LYS:CG	2.69	0.40
1:A:181:ASP:C	1:A:181:ASP:OD1	2.59	0.40
1:A:362:LYS:HD3	1:A:365:THR:OG1	2.21	0.40
1:A:208:LYS:O	1:A:209:ASP:C	2.55	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%)	3 11

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	ASP
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	37	PRO

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	327/370 (88%)	250 (76%)	77 (24%)	1 2

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	26	THR
1	A	32	HIS
1	A	38	VAL
1	A	39	ARG
1	A	42	GLN
1	A	49	GLU
1	A	51	LEU
1	A	56	VAL
1	A	60	LEU
1	A	68	LEU
1	A	74	SER
1	A	76	VAL
1	A	79	THR
1	A	80	LEU
1	A	103	PHE
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	138	SER
1	A	142	THR
1	A	159	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	166	GLU
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	225	LEU
1	A	242	THR
1	A	243	ASP
1	A	247	ARG
1	A	250	ARG
1	A	255	ASN
1	A	257	LYS
1	A	265	LYS
1	A	270	LEU
1	A	276	GLU
1	A	277	LEU
1	A	287	ILE
1	A	292	VAL
1	A	299	ASP
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	346	LYS
1	A	347	ARG
1	A	348	SER
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	384	ASN
1	A	385	GLU
1	A	399	ARG
1	A	402	THR
1	A	404	ARG
1	A	408	GLU
1	A	410	LEU
1	A	427	ARG
1	A	428	ARG
1	A	429	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
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
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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	387/439 (88%)	-0.36	5 (1%) 79 71	5, 23, 38, 47	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	GLN	3.2
1	A	428	ARG	2.9
1	A	372	ILE	2.4
1	A	430	PHE	2.4
1	A	363	LYS	2.3

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 carbohydrates 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.