



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2017 – 11:42 PM EDT

PDB ID : 5HV2
Title : Rifampin phosphotransferase G527Y mutant from *Listeria monocytogenes*
Authors : Zhang, P.; Qi, X.
Deposited on : unknown
Resolution : 2.91 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
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

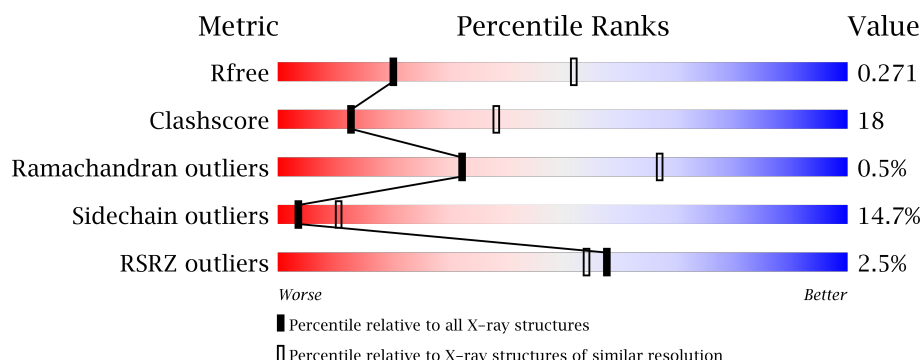
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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}	100719	1813 (2.94-2.90)
Clashscore	112137	2045 (2.94-2.90)
Ramachandran outliers	110173	1997 (2.94-2.90)
Sidechain outliers	110143	1999 (2.94-2.90)
RSRZ outliers	101464	1825 (2.94-2.90)

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	879	<div> <div>2%</div> <div>56%</div> <div>33%</div> <div>7%</div> <div>.</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6611 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 Phosphoenolpyruvate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	840	Total	C	N	O	S	0	0	0
			6610	4196	1116	1268	30			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP A0A0S2YLC8
A	-10	ARG	-	expression tag	UNP A0A0S2YLC8
A	-9	GLY	-	expression tag	UNP A0A0S2YLC8
A	-8	SER	-	expression tag	UNP A0A0S2YLC8
A	-7	HIS	-	expression tag	UNP A0A0S2YLC8
A	-6	HIS	-	expression tag	UNP A0A0S2YLC8
A	-5	HIS	-	expression tag	UNP A0A0S2YLC8
A	-4	HIS	-	expression tag	UNP A0A0S2YLC8
A	-3	HIS	-	expression tag	UNP A0A0S2YLC8
A	-2	HIS	-	expression tag	UNP A0A0S2YLC8
A	-1	GLY	-	expression tag	UNP A0A0S2YLC8
A	0	SER	-	expression tag	UNP A0A0S2YLC8
A	527	TYR	GLY	engineered mutation	UNP A0A0S2YLC8

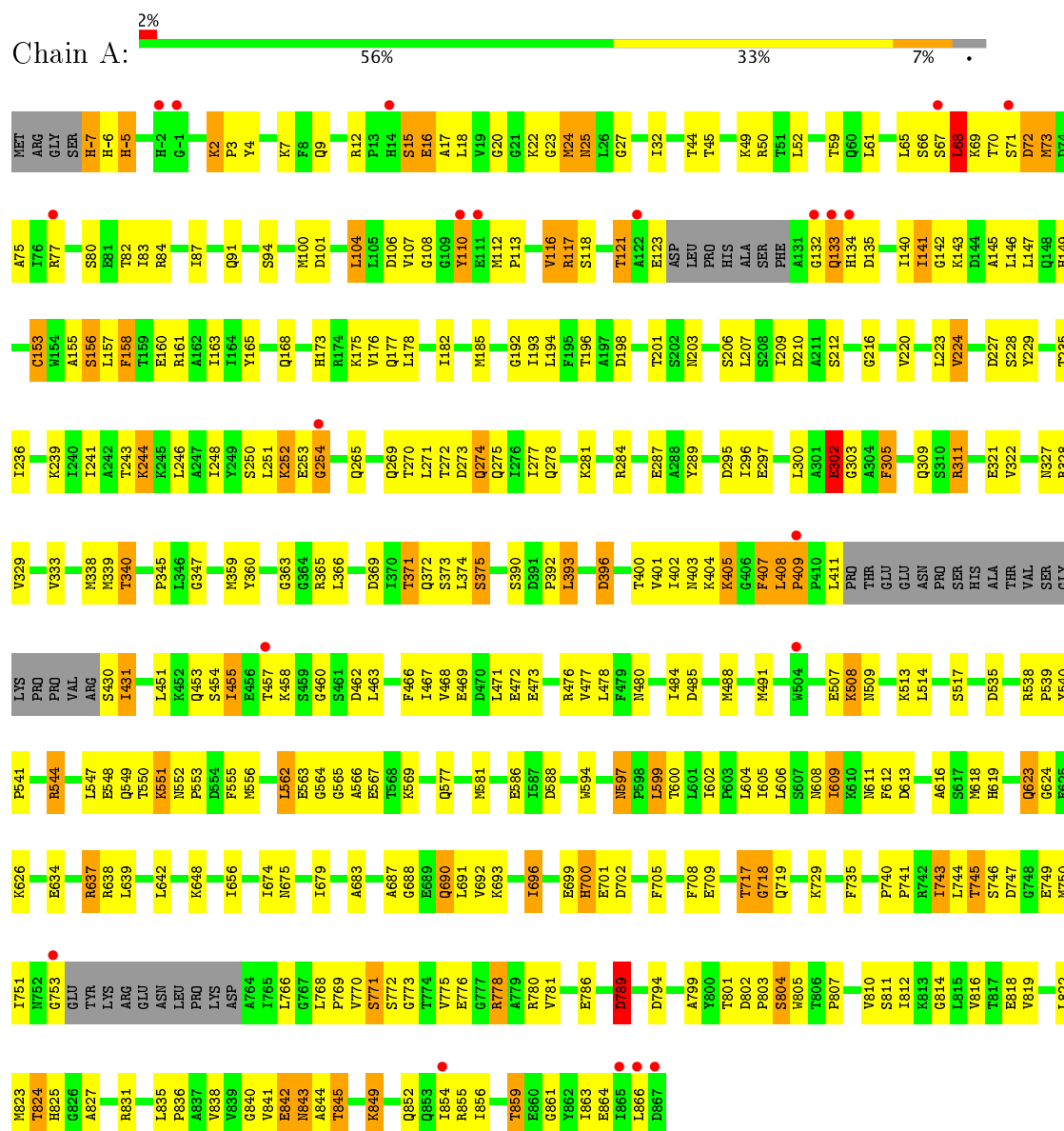
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O	0	0
			1	1		

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 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: Phosphoenolpyruvate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	58.75Å 128.76Å 142.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.40 – 2.91 43.40 – 2.91	Depositor EDS
% Data completeness (in resolution range)	91.8 (43.40-2.91) 91.9 (43.40-2.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.212 , 0.269 0.216 , 0.271	Depositor DCC
R_{free} test set	1922 reflections (8.50%)	DCC
Wilson B-factor (Å ²)	51.9	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6611	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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	0.58	1/6730 (0.0%)	0.87	22/9103 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	586	GLU	CD-OE2	-5.42	1.19	1.25

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	GLY	N-CA-C	21.21	166.13	113.10
1	A	254	GLY	C-N-CA	17.42	158.88	122.30
1	A	407	PHE	N-CA-C	11.62	142.38	111.00
1	A	407	PHE	CB-CA-C	-9.71	90.98	110.40
1	A	431	ILE	N-CA-C	8.80	134.77	111.00
1	A	789	ASP	N-CA-C	-8.33	88.51	111.00
1	A	431	ILE	CB-CA-C	-8.21	95.17	111.60
1	A	68	LEU	CB-CA-C	-7.91	95.17	110.20
1	A	718	GLY	N-CA-C	-7.51	94.33	113.10
1	A	15	SER	CB-CA-C	7.51	124.36	110.10
1	A	789	ASP	CB-CA-C	7.18	124.76	110.40
1	A	861	GLY	N-CA-C	-7.18	95.15	113.10
1	A	158	PHE	CB-CA-C	7.16	124.72	110.40
1	A	-7	HIS	C-N-CA	6.40	137.71	121.70
1	A	68	LEU	N-CA-C	6.09	127.44	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	302	GLU	N-CA-C	-6.02	94.75	111.00
1	A	597	ASN	N-CA-C	-5.62	95.83	111.00
1	A	72	ASP	CB-CA-C	-5.58	99.25	110.40
1	A	409	PRO	C-N-CD	5.47	139.90	128.40
1	A	597	ASN	CB-CA-C	5.36	121.12	110.40
1	A	340	THR	CB-CA-C	-5.31	97.26	111.60
1	A	393	LEU	CA-CB-CG	5.25	127.37	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	254	GLY	Peptide
1	A	859	THR	Peptide

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	6610	0	6637	245	1
2	A	1	0	0	0	0
All	All	6611	0	6637	245	1

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 18.

All (245) 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:431:ILE:CG2	1:A:431:ILE:O	1.91	1.15
1:A:-7:HIS:HB3	1:A:-6:HIS:HB2	1.26	1.09
1:A:72:ASP:OD1	1:A:73:MET:N	1.98	0.94
1:A:405:LYS:HE3	1:A:405:LYS:HA	1.48	0.93
1:A:431:ILE:HG22	1:A:431:ILE:O	1.13	0.92
1:A:68:LEU:HD12	1:A:68:LEU:H	1.41	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ASP:OD2	1:A:311:ARG:NH1	2.11	0.82
1:A:802:ASP:HB2	1:A:805:TRP:HD1	1.44	0.82
1:A:776:GLU:HG3	1:A:855:ARG:HG3	1.61	0.82
1:A:841:VAL:HG23	1:A:844:ALA:HB2	1.61	0.81
1:A:476:ARG:O	1:A:480:ASN:ND2	2.15	0.80
1:A:802:ASP:HB3	1:A:804:SER:H	1.46	0.80
1:A:405:LYS:HA	1:A:405:LYS:CE	2.11	0.78
1:A:244:LYS:NZ	1:A:270:THR:OG1	2.17	0.75
1:A:-7:HIS:CB	1:A:-6:HIS:HB2	2.12	0.75
1:A:133:GLN:O	1:A:134:HIS:ND1	2.20	0.73
1:A:369:ASP:OD1	1:A:371:THR:HG22	1.88	0.73
1:A:52:LEU:HD11	1:A:87:ILE:HG23	1.71	0.71
1:A:771:SER:OG	1:A:835:LEU:O	2.08	0.71
1:A:842:GLU:OE2	1:A:843:ASN:N	2.23	0.70
1:A:718:GLY:O	1:A:719:GLN:OE1	2.09	0.70
1:A:269:GLN:NE2	1:A:273:ASP:OD1	2.25	0.69
1:A:508:LYS:HD3	1:A:509:ASN:H	1.59	0.68
1:A:801:THR:HG22	1:A:825:HIS:CD2	2.29	0.68
1:A:223:LEU:HD12	1:A:799:ALA:HB1	1.75	0.67
1:A:16:GLU:HB2	1:A:24:MET:HG3	1.77	0.67
1:A:548:GLU:HG3	1:A:606:LEU:HD13	1.77	0.65
1:A:133:GLN:O	1:A:134:HIS:CG	2.50	0.65
1:A:236:ILE:HG21	1:A:239:LYS:HE3	1.77	0.65
1:A:392:PRO:O	1:A:393:LEU:HB3	1.95	0.65
1:A:468:VAL:HA	1:A:471:LEU:HD12	1.79	0.65
1:A:270:THR:HG22	1:A:271:LEU:HD13	1.79	0.64
1:A:508:LYS:HD3	1:A:509:ASN:N	2.13	0.64
1:A:20:GLY:HA2	1:A:121:THR:HG22	1.79	0.64
1:A:789:ASP:N	1:A:789:ASP:OD1	2.30	0.64
1:A:329:VAL:HG13	1:A:743:ILE:HD13	1.79	0.63
1:A:104:LEU:HD13	1:A:110:TYR:CE1	2.34	0.62
1:A:780:ARG:NH1	1:A:789:ASP:OD1	2.30	0.62
1:A:408:LEU:HD23	1:A:408:LEU:H	1.63	0.61
1:A:340:THR:O	1:A:340:THR:OG1	2.17	0.61
1:A:113:PRO:HG2	1:A:185:MET:HB2	1.82	0.61
1:A:855:ARG:NH1	1:A:864:GLU:OE1	2.34	0.61
1:A:241:ILE:HD11	1:A:269:GLN:HG3	1.83	0.60
1:A:133:GLN:HB3	1:A:161:ARG:HH11	1.66	0.60
1:A:363:GLY:HA2	1:A:735:PHE:CE1	2.37	0.60
1:A:824:THR:HG22	1:A:827:ALA:H	1.67	0.60
1:A:393:LEU:HD12	1:A:753:GLY:HA3	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ASP:HB2	1:A:206:SER:HB2	1.84	0.60
1:A:4:TYR:OH	1:A:50:ARG:NE	2.35	0.60
1:A:803:PRO:HA	1:A:825:HIS:CE1	2.37	0.59
1:A:251:LEU:HD22	1:A:252:LYS:HE3	1.84	0.59
1:A:741:PRO:HG2	1:A:744:LEU:HB2	1.85	0.59
1:A:856:ILE:HG22	1:A:863:ILE:HG23	1.83	0.59
1:A:145:ALA:O	1:A:149:HIS:ND1	2.31	0.59
1:A:297:GLU:OE1	1:A:309:GLN:NE2	2.35	0.59
1:A:104:LEU:HD13	1:A:110:TYR:CZ	2.38	0.58
1:A:73:MET:HA	1:A:73:MET:HE3	1.84	0.58
1:A:768:LEU:HD12	1:A:769:PRO:HD2	1.84	0.58
1:A:455:ILE:HG12	1:A:466:PHE:HE1	1.68	0.58
1:A:194:LEU:HD11	1:A:207:LEU:HD21	1.86	0.58
1:A:467:ILE:HD11	1:A:708:PHE:HE1	1.69	0.58
1:A:608:ASN:O	1:A:612:PHE:HB2	2.04	0.57
1:A:322:VAL:HG22	1:A:360:TYR:CD1	2.39	0.57
1:A:480:ASN:O	1:A:484:ILE:HG12	2.04	0.57
1:A:140:ILE:HD12	1:A:146:LEU:HA	1.86	0.57
1:A:72:ASP:O	1:A:73:MET:HG2	2.03	0.57
1:A:274:GLN:O	1:A:278:GLN:HB2	2.04	0.57
1:A:408:LEU:H	1:A:408:LEU:CD2	2.17	0.57
1:A:198:ASP:HB3	1:A:201:THR:HB	1.86	0.57
1:A:781:VAL:HG13	1:A:845:THR:HG22	1.86	0.57
1:A:212:SER:HB2	1:A:216:GLY:HA2	1.86	0.57
1:A:32:ILE:HG12	1:A:289:TYR:CD1	2.40	0.56
1:A:345:PRO:HG2	1:A:705:PHE:HA	1.86	0.56
1:A:780:ARG:NH1	1:A:789:ASP:O	2.40	0.55
1:A:110:TYR:HE2	1:A:143:LYS:HA	1.71	0.55
1:A:220:VAL:HG21	1:A:248:ILE:HG21	1.86	0.55
1:A:745:THR:HG23	1:A:747:ASP:H	1.72	0.55
1:A:812:ILE:HD12	1:A:814:GLY:O	2.07	0.55
1:A:822:LEU:O	1:A:831:ARG:NH2	2.39	0.55
1:A:401:VAL:HG22	1:A:751:ILE:HD12	1.89	0.54
1:A:824:THR:HG22	1:A:827:ALA:N	2.21	0.54
1:A:194:LEU:HD12	1:A:209:ILE:HG12	1.89	0.54
1:A:133:GLN:HB3	1:A:161:ARG:NH1	2.21	0.54
1:A:473:GLU:O	1:A:477:VAL:HG23	2.08	0.54
1:A:565:GLY:O	1:A:566:ALA:HB3	2.06	0.54
1:A:455:ILE:HD12	1:A:679:ILE:HG22	1.89	0.54
1:A:158:PHE:O	1:A:163:ILE:CD1	2.56	0.53
1:A:133:GLN:OE1	1:A:133:GLN:HA	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:ARG:NH2	1:A:609:ILE:HA	2.24	0.53
1:A:23:GLY:C	1:A:25:ASN:H	2.12	0.53
1:A:405:LYS:CE	1:A:405:LYS:CA	2.85	0.53
1:A:15:SER:O	1:A:18:LEU:N	2.40	0.52
1:A:535:ASP:HA	1:A:538:ARG:HD2	1.90	0.52
1:A:104:LEU:O	1:A:108:GLY:HA2	2.09	0.52
1:A:101:ASP:OD2	1:A:143:LYS:NZ	2.41	0.52
1:A:70:THR:O	1:A:71:SER:OG	2.12	0.52
1:A:201:THR:HG21	1:A:203:ASN:HB2	1.91	0.52
1:A:467:ILE:HD11	1:A:708:PHE:CE1	2.44	0.52
1:A:551:LYS:O	1:A:553:PRO:HD3	2.10	0.52
1:A:539:PRO:O	1:A:541:PRO:HD3	2.10	0.52
1:A:700:HIS:CE1	1:A:701:GLU:HG3	2.45	0.52
1:A:61:LEU:HD21	1:A:82:THR:HG22	1.91	0.51
1:A:201:THR:HG23	1:A:749:GLU:HG3	1.93	0.51
1:A:372:GLN:O	1:A:375:SER:OG	2.28	0.51
1:A:408:LEU:N	1:A:408:LEU:CD2	2.73	0.51
1:A:517:SER:OG	1:A:624:GLY:HA3	2.10	0.51
1:A:15:SER:O	1:A:17:ALA:N	2.44	0.50
1:A:69:LYS:HE2	1:A:75:ALA:HB1	1.92	0.50
1:A:702:ASP:OD1	1:A:729:LYS:NZ	2.32	0.50
1:A:717:THR:O	1:A:719:GLN:N	2.44	0.50
1:A:594:TRP:O	1:A:597:ASN:O	2.29	0.50
1:A:272:THR:O	1:A:275:GLN:N	2.45	0.49
1:A:552:ASN:O	1:A:555:PHE:HB3	2.11	0.49
1:A:605:ILE:O	1:A:609:ILE:HG22	2.13	0.49
1:A:814:GLY:HA3	1:A:856:ILE:HD11	1.94	0.49
1:A:23:GLY:O	1:A:25:ASN:N	2.46	0.49
1:A:117:ARG:HB2	1:A:117:ARG:NH1	2.28	0.49
1:A:160:GLU:OE1	1:A:160:GLU:N	2.31	0.48
1:A:691:LEU:O	1:A:696:ILE:HG22	2.13	0.48
1:A:72:ASP:C	1:A:73:MET:HG2	2.32	0.48
1:A:87:ILE:HD12	1:A:155:ALA:HA	1.95	0.48
1:A:540:TYR:CD1	1:A:564:GLY:HA2	2.49	0.48
1:A:104:LEU:HD13	1:A:110:TYR:OH	2.13	0.48
1:A:451:LEU:HD23	1:A:679:ILE:HD12	1.96	0.48
1:A:544:ARG:NH2	1:A:548:GLU:OE1	2.47	0.48
1:A:110:TYR:HE2	1:A:143:LYS:CA	2.27	0.48
1:A:284:ARG:HD3	1:A:287:GLU:OE1	2.14	0.48
1:A:4:TYR:O	1:A:44:THR:HG23	2.14	0.48
1:A:540:TYR:CG	1:A:564:GLY:HA2	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:773:GLY:HA3	1:A:836:PRO:HG3	1.96	0.48
1:A:556:MET:O	1:A:569:LYS:HD2	2.14	0.47
1:A:781:VAL:CG1	1:A:845:THR:HG22	2.44	0.47
1:A:484:ILE:O	1:A:488:MET:HG2	2.14	0.47
1:A:83:ILE:O	1:A:87:ILE:HG13	2.14	0.47
1:A:23:GLY:O	1:A:27:GLY:N	2.38	0.47
1:A:153:CYS:O	1:A:156:SER:HB3	2.15	0.47
1:A:374:LEU:HD22	1:A:402:ILE:HD11	1.95	0.47
1:A:141:ILE:HG12	1:A:142:GLY:N	2.28	0.47
1:A:454:SER:O	1:A:457:THR:HB	2.13	0.47
1:A:158:PHE:O	1:A:163:ILE:HD11	2.14	0.47
1:A:194:LEU:HD22	1:A:296:ILE:HD12	1.96	0.47
1:A:66:SER:HA	1:A:173:HIS:HD2	1.79	0.47
1:A:302:GLU:HB2	1:A:303:GLY:H	1.56	0.47
1:A:549:GLN:HG2	1:A:549:GLN:O	2.15	0.46
1:A:327:ASN:HB3	1:A:407:PHE:CE1	2.50	0.46
1:A:766:LEU:O	1:A:841:VAL:HG12	2.15	0.46
1:A:838:VAL:HG21	1:A:863:ILE:HG12	1.96	0.46
1:A:146:LEU:HD11	1:A:182:ILE:HD12	1.98	0.46
1:A:634:GLU:HA	1:A:637:ARG:NH1	2.31	0.46
1:A:68:LEU:HD12	1:A:68:LEU:N	2.20	0.46
1:A:133:GLN:CD	1:A:803:PRO:HB2	2.36	0.46
1:A:133:GLN:O	1:A:134:HIS:CE1	2.68	0.46
1:A:84:ARG:HG3	1:A:155:ALA:HB1	1.96	0.46
1:A:778:ARG:NH1	1:A:794:ASP:OD1	2.48	0.46
1:A:623:GLN:O	1:A:623:GLN:HG2	2.16	0.46
1:A:135:ASP:HB2	1:A:156:SER:HB2	1.98	0.46
1:A:140:ILE:HD11	1:A:146:LEU:HD13	1.98	0.46
1:A:547:LEU:O	1:A:550:THR:HG22	2.16	0.46
1:A:597:ASN:O	1:A:600:THR:HG22	2.17	0.45
1:A:66:SER:HA	1:A:173:HIS:CD2	2.51	0.45
1:A:113:PRO:HG2	1:A:185:MET:CB	2.46	0.45
1:A:849:LYS:O	1:A:852:GLN:HG3	2.16	0.45
1:A:514:LEU:HD13	1:A:656:ILE:HG12	1.99	0.45
1:A:451:LEU:HD11	1:A:455:ILE:HD11	1.98	0.45
1:A:801:THR:CG2	1:A:825:HIS:CD2	3.00	0.44
1:A:333:VAL:HG21	1:A:359:MET:HE2	1.99	0.44
1:A:404:LYS:HE2	1:A:404:LYS:HB3	1.67	0.44
1:A:116:VAL:HG21	1:A:140:ILE:HD13	1.99	0.44
1:A:277:ILE:O	1:A:281:LYS:HG3	2.17	0.44
1:A:360:TYR:HE2	1:A:369:ASP:HB2	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:VAL:HG21	1:A:863:ILE:CG1	2.47	0.44
1:A:157:LEU:HD21	1:A:176:VAL:HG13	2.00	0.44
1:A:61:LEU:HA	1:A:61:LEU:HD12	1.75	0.44
1:A:745:THR:CG2	1:A:747:ASP:H	2.29	0.44
1:A:322:VAL:HG13	1:A:360:TYR:CZ	2.52	0.44
1:A:562:LEU:HG	1:A:562:LEU:H	1.55	0.44
1:A:818:GLU:O	1:A:840:GLY:HA2	2.18	0.44
1:A:-7:HIS:N	1:A:-5:HIS:H	2.16	0.43
1:A:408:LEU:N	1:A:408:LEU:HD23	2.28	0.43
1:A:457:THR:HG22	1:A:458:LYS:HD2	2.00	0.43
1:A:49:LYS:HE3	1:A:177:GLN:NE2	2.33	0.43
1:A:565:GLY:O	1:A:567:GLU:N	2.44	0.43
1:A:599:LEU:HD12	1:A:602:ILE:HD12	2.00	0.43
1:A:674:ILE:HA	1:A:674:ILE:HD13	1.70	0.43
1:A:216:GLY:O	1:A:220:VAL:HG12	2.18	0.43
1:A:327:ASN:HB3	1:A:407:PHE:CZ	2.54	0.43
1:A:687:ALA:O	1:A:691:LEU:HD13	2.19	0.43
1:A:859:THR:HG22	1:A:859:THR:O	2.19	0.43
1:A:107:VAL:H	1:A:108:GLY:HA3	1.82	0.43
1:A:469:GLU:O	1:A:472:GLU:HB2	2.19	0.43
1:A:623:GLN:HA	1:A:626:LYS:HB3	2.00	0.43
1:A:709:GLU:H	1:A:709:GLU:CD	2.23	0.43
1:A:73:MET:HA	1:A:73:MET:CE	2.49	0.43
1:A:84:ARG:CG	1:A:155:ALA:HB1	2.49	0.43
1:A:463:LEU:HD21	1:A:683:ALA:HB1	2.01	0.42
1:A:648:LYS:HB3	1:A:648:LYS:HE2	1.73	0.42
1:A:802:ASP:HB3	1:A:804:SER:HB3	2.01	0.42
1:A:396:ASP:N	1:A:396:ASP:OD2	2.51	0.42
1:A:-5:HIS:ND1	1:A:-5:HIS:N	2.66	0.42
1:A:80:SER:O	1:A:84:ARG:HB2	2.19	0.42
1:A:192:GLY:HA3	1:A:210:ASP:O	2.19	0.42
1:A:717:THR:OG1	1:A:719:GLN:HB2	2.19	0.42
1:A:157:LEU:HD13	1:A:178:LEU:HG	2.02	0.42
1:A:100:MET:O	1:A:104:LEU:HD12	2.19	0.42
1:A:616:ALA:HA	1:A:619:HIS:HB2	2.01	0.42
1:A:849:LYS:HB2	1:A:852:GLN:NE2	2.35	0.42
1:A:123:GLU:HB2	1:A:175:LYS:HD3	2.01	0.42
1:A:227:ASP:HB3	1:A:229:TYR:CE1	2.54	0.42
1:A:345:PRO:HG2	1:A:705:PHE:C	2.40	0.42
1:A:347:GLY:HA3	1:A:588:ASP:OD1	2.20	0.42
1:A:594:TRP:HD1	1:A:600:THR:HG23	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:SER:OG	1:A:84:ARG:NH1	2.50	0.42
1:A:224:VAL:O	1:A:819:VAL:HG23	2.20	0.42
1:A:16:GLU:O	1:A:16:GLU:HG3	2.20	0.41
1:A:717:THR:OG1	1:A:719:GLN:OE1	2.29	0.41
1:A:799:ALA:HA	1:A:818:GLU:HG3	2.01	0.41
1:A:2:LYS:HA	1:A:3:PRO:HD3	1.68	0.41
1:A:463:LEU:HD11	1:A:683:ALA:HB1	2.02	0.41
1:A:822:LEU:HA	1:A:822:LEU:HD23	1.88	0.41
1:A:300:LEU:HD13	1:A:305:PHE:CE1	2.56	0.41
1:A:107:VAL:H	1:A:108:GLY:CA	2.33	0.41
1:A:201:THR:CG2	1:A:203:ASN:HB2	2.51	0.41
1:A:634:GLU:HG2	1:A:638:ARG:HD3	2.03	0.41
1:A:696:ILE:O	1:A:696:ILE:HD12	2.20	0.41
1:A:132:GLY:HA3	1:A:165:TYR:CE2	2.55	0.41
1:A:604:LEU:HD12	1:A:604:LEU:H	1.85	0.41
1:A:365:ARG:HD3	1:A:740:PRO:HG3	2.03	0.41
1:A:639:LEU:O	1:A:642:LEU:HB2	2.20	0.40
1:A:393:LEU:CD1	1:A:753:GLY:HA3	2.50	0.40
1:A:107:VAL:N	1:A:108:GLY:HA3	2.37	0.40
1:A:16:GLU:CB	1:A:24:MET:HG3	2.48	0.40
1:A:675:ASN:O	1:A:679:ILE:HG13	2.21	0.40
1:A:688:GLY:O	1:A:692:VAL:HG23	2.21	0.40
1:A:786:GLU:CD	1:A:786:GLU:H	2.24	0.40
1:A:818:GLU:OE2	1:A:845:THR:OG1	2.38	0.40
1:A:196:THR:HA	1:A:207:LEU:HD12	2.03	0.40
1:A:23:GLY:C	1:A:25:ASN:N	2.74	0.40
1:A:328:ARG:HB3	1:A:371:THR:HG21	2.02	0.40
1:A:366:LEU:HD23	1:A:366:LEU:HA	1.86	0.40
1:A:597:ASN:OD1	1:A:599:LEU:HB2	2.22	0.40
1:A:690:GLN:NE2	1:A:693:LYS:HE3	2.36	0.40
1:A:69:LYS:HE2	1:A:75:ALA:CB	2.50	0.40
1:A:802:ASP:HB2	1:A:805:TRP:CD1	2.37	0.40
1:A:816:VAL:HG22	1:A:838:VAL:HG23	2.04	0.40
1:A:107:VAL:N	1:A:108:GLY:CA	2.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ARG:NH1	1:A:485:ASP:OD2[3_755]	2.17	0.03

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	832/879 (95%)	753 (90%)	75 (9%)	4 (0%)	32 67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	MET
1	A	460	GLY
1	A	409	PRO
1	A	807	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	721/757 (95%)	615 (85%)	106 (15%)	3 11

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-5	HIS
1	A	2	LYS
1	A	7	LYS
1	A	9	GLN
1	A	16	GLU
1	A	22	LYS
1	A	25	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	45	THR
1	A	59	THR
1	A	65	LEU
1	A	67	SER
1	A	68	LEU
1	A	73	MET
1	A	77	ARG
1	A	91	GLN
1	A	94	SER
1	A	104	LEU
1	A	106	ASP
1	A	110	TYR
1	A	112	MET
1	A	116	VAL
1	A	117	ARG
1	A	118	SER
1	A	121	THR
1	A	133	GLN
1	A	141	ILE
1	A	147	LEU
1	A	153	CYS
1	A	156	SER
1	A	168	GLN
1	A	193	ILE
1	A	224	VAL
1	A	228	SER
1	A	235	THR
1	A	243	THR
1	A	244	LYS
1	A	246	LEU
1	A	250	SER
1	A	252	LYS
1	A	253	GLU
1	A	265	GLN
1	A	274	GLN
1	A	302	GLU
1	A	305	PHE
1	A	311	ARG
1	A	321	GLU
1	A	338	MET
1	A	339	MET
1	A	371	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	373	SER
1	A	375	SER
1	A	390	SER
1	A	396	ASP
1	A	400	THR
1	A	403	ASN
1	A	405	LYS
1	A	408	LEU
1	A	411	LEU
1	A	430	SER
1	A	453	GLN
1	A	455	ILE
1	A	462	ASP
1	A	478	LEU
1	A	491	MET
1	A	507	GLU
1	A	508	LYS
1	A	513	LYS
1	A	544	ARG
1	A	551	LYS
1	A	562	LEU
1	A	563	GLU
1	A	577	GLN
1	A	581	MET
1	A	599	LEU
1	A	609	ILE
1	A	611	ASN
1	A	613	ASP
1	A	618	MET
1	A	623	GLN
1	A	637	ARG
1	A	690	GLN
1	A	696	ILE
1	A	699	GLU
1	A	700	HIS
1	A	717	THR
1	A	743	ILE
1	A	745	THR
1	A	746	SER
1	A	750	MET
1	A	770	VAL
1	A	771	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	772	SER
1	A	775	VAL
1	A	778	ARG
1	A	789	ASP
1	A	804	SER
1	A	810	VAL
1	A	811	SER
1	A	823	MET
1	A	824	THR
1	A	842	GLU
1	A	843	ASN
1	A	845	THR
1	A	849	LYS
1	A	854	ILE
1	A	866	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	ASN
1	A	309	GLN
1	A	480	ASN
1	A	825	HIS

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 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	840/879 (95%)	0.14	21 (2%) 58 54	18, 47, 76, 97	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	865	ILE	3.6
1	A	867	ASP	3.4
1	A	110	TYR	3.1
1	A	409	PRO	3.0
1	A	71	SER	2.9
1	A	866	LEU	2.7
1	A	254	GLY	2.7
1	A	-2	HIS	2.7
1	A	67	SER	2.7
1	A	122	ALA	2.4
1	A	134	HIS	2.4
1	A	111	GLU	2.4
1	A	14	HIS	2.3
1	A	133	GLN	2.3
1	A	504	TRP	2.2
1	A	457	THR	2.2
1	A	753	GLY	2.2
1	A	132	GLY	2.1
1	A	854	ILE	2.1
1	A	-1	GLY	2.1
1	A	77	ARG	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 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.