Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 12:42 AM EDT

PDB ID	:	1M41
Title	:	Crystal structure of Escherichia coli alkanesulfonate monooxygenase SsuD at 2.3 A resolution
Authors	:	Eichhorn, E.; Davey, C.A.; Sargent, D.F.; Leisinger, T.; Richmond, T.J.
Deposited on	:	2002-07-02
Resolution	:	2.30 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 (i) 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 (i)) were used in the production of this report:

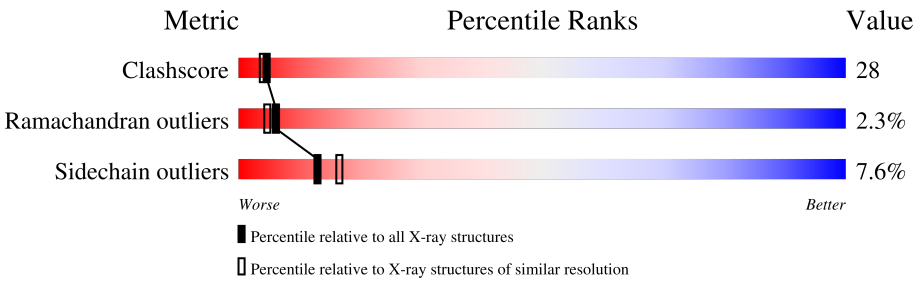
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	380	47% 36% • 14%
1	B	380	49% 33% • 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5408 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 FMNH2-dependent alkanesulfonate monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	328	2549	1628	450	468	3	0	0	0
1	B	328	2549	1628	450	468	3	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	144	144	144	0	0
2	B	166	166	166	0	0

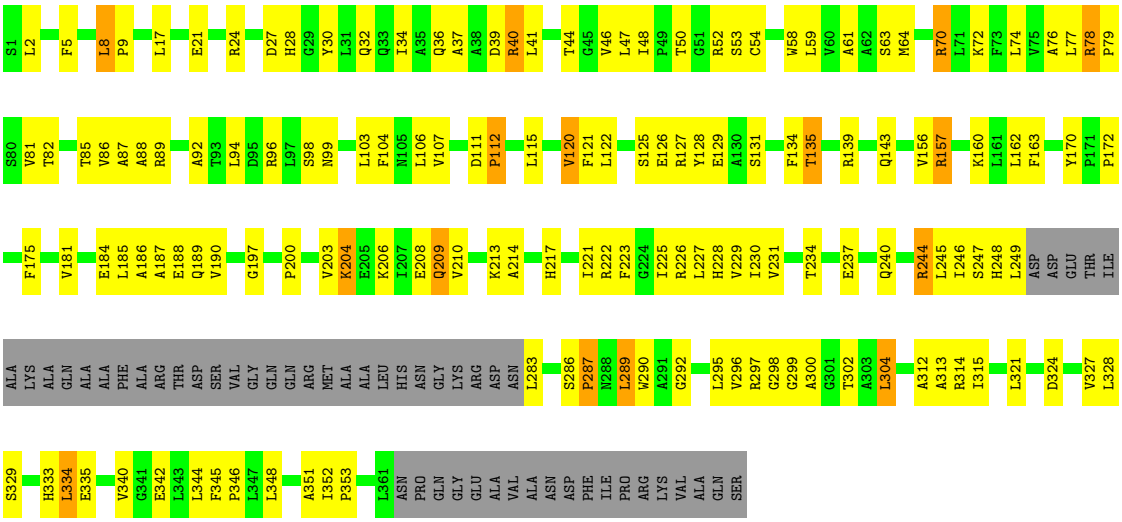
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

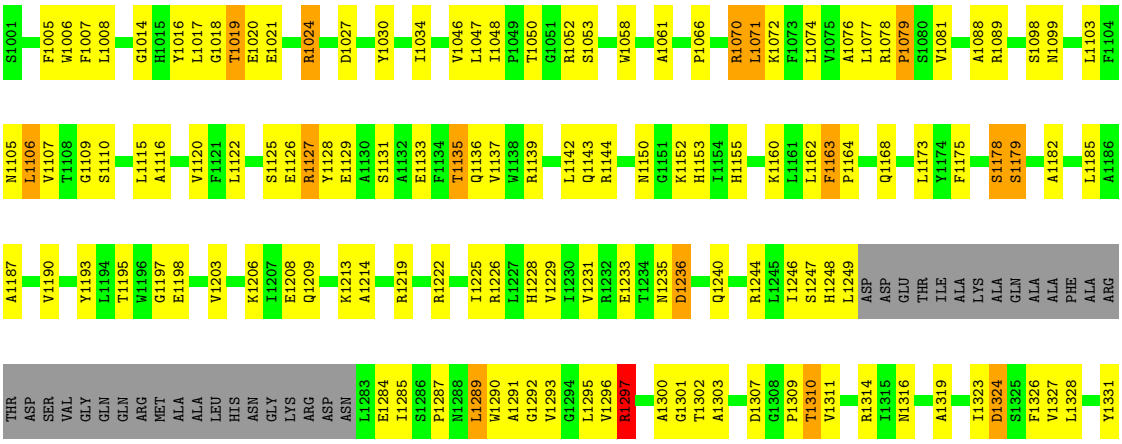
• Molecule 1: FMNH2-dependent alkanesulfonate monooxygenase

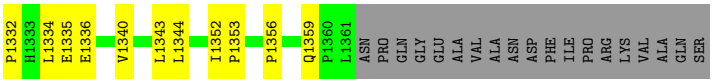
Chain A: 47% 36% • 14%



• Molecule 1: FMNH2-dependent alkanesulfonate monooxygenase

Chain B: 49% 33% • 14%




P1332
H1333
L1334
E1335
E1336
V1340
L1343
L1344
I1352
P1353
P1356
Q1359
P1360
L1361
ASN
PRO
GLN
GLY
GLU
ALA
VAL
ALA
ASN
ASP
PHE
ILE
PRO
ARG
LYS
VAL
ALA
GLN
SER

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	116.35Å 140.76Å 125.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30	Depositor
% Data completeness (in resolution range)	94.4 (25.00-2.30)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5408	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	0.54	0/2612	0.79	2/3559 (0.1%)
1	B	0.54	0/2612	0.80	2/3559 (0.1%)
All	All	0.54	0/5224	0.80	4/7118 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1071	LEU	CA-CB-CG	7.75	133.13	115.30
1	A	334	LEU	CA-CB-CG	6.49	130.23	115.30
1	A	77	LEU	CA-CB-CG	5.85	128.75	115.30
1	B	1103	LEU	CA-CB-CG	5.10	127.03	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2549	0	2526	165	0
1	B	2549	0	2523	132	0
2	A	144	0	0	9	0
2	B	166	0	0	11	0
All	All	5408	0	5049	286	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 28.

All (286) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1246:ILE:HG13	1:B:1249:LEU:HD12	1.39	1.03
1:B:1340:VAL:HG13	1:B:1344:LEU:HD12	1.41	0.98
1:A:246:ILE:HG23	1:A:249:LEU:HD12	1.50	0.93
1:A:240:GLN:O	1:A:244:ARG:HG2	1.73	0.87
1:B:1222:ARG:HD2	1:B:1324:ASP:OD2	1.76	0.85
1:B:1229:VAL:CG1	1:B:1231:VAL:HG23	2.05	0.85
1:A:344:LEU:HD21	1:A:348:LEU:HD12	1.59	0.84
1:B:1127:ARG:HH11	1:B:1127:ARG:HB3	1.41	0.83
1:A:111:ASP:HB2	1:A:112:PRO:HA	1.61	0.82
1:A:287:PRO:HB2	1:A:314:ARG:HH12	1.43	0.82
1:B:1300:ALA:O	1:B:1302:THR:N	2.12	0.81
1:A:197:GLY:HA2	1:A:225:ILE:HD11	1.63	0.81
1:B:1178:SER:HA	1:B:1193:TYR:OH	1.82	0.80
1:B:1307:ASP:OD1	1:B:1310:THR:HG22	1.83	0.78
1:B:1081:VAL:HG12	1:B:1120:VAL:HG21	1.63	0.78
1:A:115:LEU:HB3	1:A:120:VAL:HG22	1.66	0.78
1:A:125:SER:O	1:A:129:GLU:HG3	1.84	0.77
1:B:1185:LEU:HD23	1:B:1185:LEU:O	1.85	0.76
1:A:186:ALA:O	1:A:190:VAL:HG22	1.86	0.76
1:B:1024:ARG:NH1	1:B:1335:GLU:OE2	2.18	0.76
1:B:1226:ARG:NH1	2:B:296:HOH:O	2.19	0.75
1:B:1197:GLY:HA2	1:B:1225:ILE:HD11	1.70	0.74
1:A:227:LEU:HD22	1:A:304:LEU:HD13	1.69	0.74
1:B:1246:ILE:HG13	1:B:1249:LEU:CD1	2.16	0.74
1:B:1206:LYS:HA	1:B:1209:GLN:HG2	1.69	0.74
1:A:344:LEU:C	1:A:344:LEU:HD23	2.10	0.73
1:A:234:THR:OG1	1:A:237:GLU:HG3	1.89	0.72
1:A:162:LEU:HD12	1:B:1053:SER:HA	1.72	0.71
1:B:1231:VAL:HG22	1:B:1311:VAL:HG21	1.71	0.71
1:B:1099:ASN:HD22	1:B:1356:PRO:HG2	1.55	0.70
1:B:1079:PRO:HD2	1:B:1107:VAL:O	1.91	0.70
1:B:1307:ASP:CG	1:B:1310:THR:HG22	2.12	0.70
1:A:44:THR:HA	1:A:353:PRO:CG	2.20	0.70
1:A:287:PRO:HB2	1:A:314:ARG:NH1	2.07	0.70
1:B:1135:THR:O	1:B:1139:ARG:HG3	1.91	0.69
1:B:1089:ARG:HH11	1:B:1089:ARG:HB2	1.57	0.69
1:B:1122:LEU:HB3	1:B:1126:GLU:HB2	1.74	0.69
1:A:353:PRO:HB3	2:A:407:HOH:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:PRO:O	1:A:203:VAL:HG12	1.93	0.68
1:A:81:VAL:HG23	1:A:82:THR:HG23	1.74	0.68
1:A:86:VAL:HG23	1:A:87:ALA:N	2.08	0.68
1:B:1008:LEU:HD13	1:B:1046:VAL:HG11	1.75	0.68
1:B:1175:PHE:HB2	1:B:1190:VAL:HG11	1.76	0.68
1:A:208:GLU:OE2	1:A:208:GLU:HA	1.94	0.68
1:A:157:ARG:HG2	1:A:157:ARG:HH11	1.60	0.67
1:A:244:ARG:NH1	1:A:244:ARG:HA	2.09	0.67
1:A:44:THR:HA	1:A:353:PRO:HG2	1.76	0.66
1:A:53:SER:HA	1:B:1162:LEU:HD12	1.77	0.66
1:B:1127:ARG:HH11	1:B:1127:ARG:CB	2.07	0.66
1:A:226:ARG:HG2	1:A:226:ARG:HH11	1.59	0.66
1:A:227:LEU:HD13	1:A:304:LEU:CD2	2.26	0.66
1:A:27:ASP:HB2	2:A:459:HOH:O	1.95	0.66
1:A:160:LYS:H	1:B:1052:ARG:HH22	1.44	0.66
1:B:1150:ASN:HB2	1:B:1155:HIS:ND1	2.12	0.65
1:B:1229:VAL:HG12	1:B:1231:VAL:HG23	1.78	0.65
1:A:131:SER:O	1:A:135:THR:HG23	1.97	0.65
1:A:344:LEU:HD23	1:A:345:PHE:N	2.12	0.64
1:B:1125:SER:O	1:B:1129:GLU:HG2	1.96	0.64
1:B:1133:GLU:O	1:B:1137:VAL:HG23	1.96	0.64
1:A:246:ILE:O	1:A:248:HIS:N	2.30	0.64
1:B:1048:ILE:HD12	1:B:1061:ALA:HB2	1.80	0.63
1:A:40:ARG:HH11	1:A:40:ARG:HB2	1.62	0.63
1:B:1115:LEU:HB3	1:B:1120:VAL:HB	1.81	0.63
1:B:1131:SER:O	1:B:1135:THR:HG23	1.99	0.63
1:A:187:ALA:HB1	1:A:214:ALA:HA	1.80	0.63
1:A:203:VAL:HG13	1:A:321:LEU:CD1	2.29	0.63
1:B:1136:GLN:HG2	2:B:264:HOH:O	1.99	0.62
1:A:292:GLY:O	1:A:295:LEU:HD13	1.99	0.62
1:A:111:ASP:CB	1:A:112:PRO:HA	2.29	0.62
1:A:160:LYS:H	1:B:1052:ARG:NH2	1.98	0.62
1:B:1292:GLY:O	1:B:1295:LEU:HB2	2.00	0.61
1:A:58:TRP:CH2	1:A:104:PHE:HE2	2.19	0.61
1:A:344:LEU:HD21	1:A:348:LEU:CD1	2.28	0.61
1:A:227:LEU:HD13	1:A:304:LEU:HD22	1.82	0.61
1:B:1024:ARG:HH12	1:B:1335:GLU:CD	2.04	0.61
1:B:1070:ARG:HD3	2:B:2:HOH:O	2.01	0.61
1:B:1127:ARG:HG3	1:B:1128:TYR:N	2.15	0.60
1:A:287:PRO:O	1:A:314:ARG:NH1	2.35	0.60
1:B:1129:GLU:O	1:B:1133:GLU:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1058:TRP:HZ2	1:B:1077:LEU:HD13	1.67	0.60
1:A:127:ARG:HH11	1:A:127:ARG:HB2	1.66	0.60
1:A:127:ARG:HB2	1:A:127:ARG:NH1	2.17	0.60
1:A:58:TRP:CH2	1:A:104:PHE:CE2	2.90	0.59
1:A:283:LEU:HD13	1:A:292:GLY:HA2	1.83	0.59
1:A:52:ARG:HH21	1:B:1160:LYS:H	1.50	0.59
1:A:127:ARG:HH11	1:A:127:ARG:CB	2.15	0.59
1:A:21:GLU:HG2	1:A:248:HIS:CE1	2.38	0.59
1:A:290:TRP:CZ2	1:A:292:GLY:HA3	2.37	0.59
1:A:72:LYS:HE2	2:A:396:HOH:O	2.02	0.59
1:A:40:ARG:HB2	1:A:40:ARG:NH1	2.17	0.58
1:B:1008:LEU:HD13	1:B:1046:VAL:CG1	2.33	0.58
1:B:1014:GLY:O	1:B:1331:TYR:HB3	2.02	0.58
1:B:1187:ALA:HB1	1:B:1214:ALA:HA	1.86	0.58
1:A:92:ALA:O	1:A:96:ARG:HG3	2.04	0.57
1:A:162:LEU:HD12	1:B:1053:SER:CA	2.34	0.57
1:A:139:ARG:NH1	1:A:189:GLN:HG2	2.19	0.57
1:A:206:LYS:O	1:A:210:VAL:HG23	2.04	0.57
1:A:203:VAL:HG13	1:A:321:LEU:HD12	1.85	0.57
1:A:86:VAL:HG23	1:A:87:ALA:H	1.69	0.57
1:B:1287:PRO:O	1:B:1314:ARG:NH1	2.38	0.57
1:B:1020:GLU:H	1:B:1020:GLU:CD	2.07	0.57
1:B:1122:LEU:HB3	1:B:1126:GLU:CB	2.34	0.57
1:B:1018:GLY:O	1:B:1019:THR:HB	2.04	0.56
1:A:226:ARG:HD2	1:A:327:VAL:O	2.05	0.56
1:A:290:TRP:CE2	1:A:292:GLY:HA3	2.41	0.56
1:A:24:ARG:NH2	1:A:335:GLU:OE1	2.34	0.56
1:A:76:ALA:HB2	2:A:403:HOH:O	2.06	0.56
1:A:81:VAL:HG12	1:A:120:VAL:HG11	1.88	0.56
1:B:1077:LEU:O	1:B:1079:PRO:HD3	2.06	0.55
1:B:1115:LEU:HD22	1:B:1115:LEU:H	1.72	0.55
1:A:187:ALA:HB1	1:A:214:ALA:CA	2.36	0.55
1:B:1297:ARG:HG3	1:B:1297:ARG:HH11	1.71	0.55
1:B:1020:GLU:CD	1:B:1020:GLU:N	2.60	0.54
1:B:1072:LYS:HG3	2:B:104:HOH:O	2.07	0.54
1:B:1352:ILE:HD12	1:B:1352:ILE:O	2.07	0.54
1:B:1078:ARG:NH2	1:B:1081:VAL:HG21	2.21	0.54
1:A:54:CYS:O	1:B:1163:PHE:HZ	1.91	0.54
1:B:1228:HIS:HB3	1:B:1303:ALA:HB2	1.90	0.54
1:B:1178:SER:HA	1:B:1193:TYR:HH	1.72	0.54
1:B:1235:ASN:ND2	1:B:1307:ASP:OD2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1206:LYS:HA	1:B:1209:GLN:HE21	1.73	0.54
1:A:5:PHE:HB2	1:A:327:VAL:HA	1.91	0.53
1:A:50:THR:HB	1:A:76:ALA:CB	2.38	0.53
1:A:44:THR:HA	1:A:353:PRO:HG3	1.91	0.53
1:A:106:LEU:HB2	1:A:175:PHE:HD1	1.72	0.53
1:B:1291:ALA:HB1	2:B:204:HOH:O	2.08	0.53
1:A:115:LEU:HB3	1:A:120:VAL:CG2	2.37	0.53
1:B:1209:GLN:O	1:B:1213:LYS:HG3	2.08	0.53
1:B:1139:ARG:O	1:B:1143:GLN:HG3	2.09	0.52
1:A:120:VAL:CG2	1:A:120:VAL:O	2.56	0.52
1:B:1225:ILE:HG22	1:B:1323:ILE:HG21	1.90	0.52
1:A:24:ARG:HH12	1:A:335:GLU:CD	2.13	0.52
1:A:17:LEU:HG	1:A:245:LEU:HD11	1.91	0.52
1:A:289:LEU:HD21	1:A:302:THR:HB	1.92	0.52
1:B:1297:ARG:O	1:B:1297:ARG:HG2	2.10	0.52
1:B:1079:PRO:CD	1:B:1107:VAL:O	2.57	0.51
1:B:1089:ARG:HB2	1:B:1089:ARG:NH1	2.25	0.51
1:A:86:VAL:CG2	1:A:87:ALA:N	2.73	0.51
1:B:1236:ASP:O	1:B:1240:GLN:HG3	2.11	0.51
1:A:85:THR:O	1:A:88:ALA:N	2.42	0.51
1:B:1340:VAL:O	1:B:1344:LEU:HB2	2.11	0.51
1:B:1353:PRO:HA	2:B:300:HOH:O	2.10	0.51
1:A:96:ARG:NH1	1:A:163:PHE:HB2	2.25	0.50
1:A:121:PHE:O	1:A:122:LEU:HD23	2.12	0.50
1:A:340:VAL:HG13	1:A:344:LEU:HD13	1.93	0.50
1:A:289:LEU:CD2	1:A:302:THR:HB	2.41	0.50
1:B:1284:GLU:O	1:B:1284:GLU:HG2	2.10	0.50
1:B:1126:GLU:HA	1:B:1129:GLU:HG2	1.93	0.50
1:A:32:GLN:O	1:A:36:GLN:HB2	2.12	0.50
1:B:1129:GLU:HG3	1:B:1153:HIS:NE2	2.27	0.50
1:A:228:HIS:ND1	1:A:329:SER:OG	2.43	0.50
1:A:227:LEU:HD13	1:A:304:LEU:HD21	1.93	0.49
1:B:1030:TYR:CE1	1:B:1034:ILE:HD11	2.47	0.49
1:A:227:LEU:O	1:A:328:LEU:HA	2.13	0.49
1:B:1089:ARG:NH1	1:B:1089:ARG:CB	2.75	0.49
1:B:1106:LEU:HD11	1:B:1173:LEU:HD11	1.94	0.49
1:A:204:LYS:O	1:A:208:GLU:HG2	2.13	0.49
1:B:1187:ALA:HB1	1:B:1214:ALA:CA	2.42	0.49
1:B:1228:HIS:CD2	1:B:1293:VAL:HG11	2.47	0.49
1:A:86:VAL:CG2	1:A:87:ALA:H	2.25	0.49
1:A:37:ALA:O	1:A:40:ARG:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ARG:O	1:A:143:GLN:HG3	2.12	0.49
1:A:106:LEU:HD11	1:A:135:THR:HG21	1.95	0.48
1:A:128:TYR:HB3	1:A:181:VAL:HG11	1.95	0.48
1:B:1187:ALA:O	1:B:1219:ARG:HD3	2.12	0.48
1:B:1246:ILE:O	1:B:1248:HIS:N	2.46	0.48
1:A:78:ARG:HH21	1:A:78:ARG:HB3	1.76	0.48
1:A:160:LYS:N	1:B:1052:ARG:HH22	2.11	0.48
1:A:139:ARG:HG2	1:A:170:TYR:CE2	2.49	0.48
1:B:1127:ARG:HB3	1:B:1127:ARG:NH1	2.19	0.48
1:B:1290:TRP:O	1:B:1302:THR:HA	2.14	0.48
1:A:78:ARG:HH21	1:A:78:ARG:CB	2.26	0.48
1:A:230:ILE:HG22	1:A:230:ILE:O	2.13	0.48
1:A:286:SER:O	1:A:287:PRO:C	2.52	0.48
1:B:1326:PHE:HB3	1:B:1328:LEU:HD21	1.94	0.48
1:B:1290:TRP:CE2	1:B:1292:GLY:HA3	2.48	0.48
1:A:28:HIS:HE1	1:B:1066:PRO:HB3	1.79	0.47
1:B:1016:TYR:HE1	1:B:1244:ARG:HG2	1.79	0.47
1:A:47:LEU:HA	1:A:74:LEU:HB3	1.97	0.47
1:A:85:THR:HG22	1:A:89:ARG:NH1	2.30	0.47
1:A:226:ARG:HG2	1:A:226:ARG:NH1	2.27	0.47
1:B:1115:LEU:H	1:B:1115:LEU:CD2	2.27	0.47
1:A:85:THR:HG22	1:A:89:ARG:HH12	1.80	0.47
1:A:228:HIS:CD2	1:A:300:ALA:HB3	2.50	0.47
1:B:1316:ASN:O	1:B:1319:ALA:N	2.48	0.47
1:B:1116:ALA:HB2	2:B:220:HOH:O	2.13	0.47
1:A:184:GLU:OE2	1:A:217:HIS:CE1	2.68	0.47
1:B:1047:LEU:HA	1:B:1074:LEU:HB3	1.97	0.47
1:A:188:GLU:HG2	1:A:189:GLN:HG3	1.97	0.46
1:A:70:ARG:HD3	2:A:391:HOH:O	2.15	0.46
1:B:1089:ARG:HH11	1:B:1089:ARG:CB	2.26	0.46
1:A:47:LEU:HD23	1:A:327:VAL:HG11	1.98	0.46
1:A:126:GLU:O	1:A:129:GLU:HB2	2.16	0.46
1:A:157:ARG:HG2	1:A:157:ARG:NH1	2.30	0.45
1:B:1206:LYS:HE3	2:B:183:HOH:O	2.14	0.45
1:B:1179:SER:HB2	1:B:1182:ALA:CB	2.46	0.45
1:A:287:PRO:C	1:A:314:ARG:HH12	2.19	0.45
1:A:50:THR:HG21	1:A:107:VAL:HG21	1.97	0.45
1:A:8:LEU:HD12	1:A:8:LEU:HA	1.74	0.45
1:A:63:SER:OG	1:A:64:MET:HE2	2.17	0.45
1:A:190:VAL:HG23	1:A:221:ILE:HD11	1.98	0.45
1:A:344:LEU:C	1:A:344:LEU:CD2	2.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ILE:O	1:A:37:ALA:HB3	2.17	0.45
1:A:81:VAL:CG2	1:A:82:THR:HG23	2.45	0.45
1:B:1018:GLY:O	1:B:1019:THR:CB	2.65	0.45
1:B:1050:THR:HB	1:B:1076:ALA:HB3	1.99	0.45
1:A:21:GLU:HG2	1:A:248:HIS:HE1	1.81	0.44
1:A:86:VAL:HG12	1:A:89:ARG:NH2	2.32	0.44
1:B:1206:LYS:HA	1:B:1209:GLN:NE2	2.32	0.44
1:A:28:HIS:CD2	1:A:64:MET:CE	2.99	0.44
1:A:175:PHE:HD2	1:A:186:ALA:HB2	1.82	0.44
1:B:1152:LYS:HG3	2:B:301:HOH:O	2.17	0.44
1:B:1289:LEU:HD23	1:B:1289:LEU:HA	1.70	0.44
1:B:1307:ASP:OD1	1:B:1309:PRO:HG2	2.17	0.44
1:A:121:PHE:CE1	1:B:1155:HIS:CD2	3.05	0.44
1:A:312:ALA:O	1:A:315:ILE:HB	2.18	0.44
1:B:1179:SER:HB2	1:B:1182:ALA:HB3	2.00	0.44
1:B:1297:ARG:HG3	1:B:1297:ARG:NH1	2.32	0.44
1:B:1296:VAL:HG12	1:B:1297:ARG:N	2.32	0.44
1:A:39:ASP:O	1:A:70:ARG:NH1	2.47	0.44
1:A:244:ARG:HA	1:A:244:ARG:HH11	1.80	0.44
1:B:1005:PHE:HB2	1:B:1327:VAL:HA	1.99	0.44
1:B:1115:LEU:HD22	1:B:1115:LEU:N	2.31	0.44
1:B:1178:SER:O	1:B:1179:SER:C	2.55	0.44
1:A:79:PRO:HA	1:A:134:PHE:CD1	2.52	0.43
1:A:98:SER:O	1:A:99:ASN:HB3	2.18	0.43
1:A:299:GLY:HA2	2:A:436:HOH:O	2.18	0.43
1:A:30:TYR:CE1	1:A:34:ILE:HD11	2.53	0.43
1:A:229:VAL:HG12	1:A:230:ILE:N	2.33	0.43
1:A:5:PHE:HB2	1:A:327:VAL:HG22	2.00	0.43
1:A:120:VAL:O	1:A:120:VAL:HG23	2.18	0.43
1:B:1006:TRP:CG	1:B:1007:PHE:N	2.87	0.43
1:A:228:HIS:CE1	1:A:329:SER:HG	2.35	0.43
1:B:1296:VAL:CG1	1:B:1297:ARG:N	2.81	0.43
1:A:229:VAL:CG1	1:A:230:ILE:N	2.82	0.43
1:B:1088:ALA:HB1	1:B:1142:LEU:CD2	2.49	0.43
1:B:1099:ASN:ND2	1:B:1356:PRO:HG2	2.27	0.43
1:A:222:ARG:HD2	1:A:324:ASP:OD2	2.18	0.42
1:A:327:VAL:O	1:A:327:VAL:HG12	2.18	0.42
1:B:1198:GLU:HB2	1:B:1203:VAL:HG23	2.01	0.42
1:A:28:HIS:CD2	1:A:64:MET:HE2	2.54	0.42
1:A:342:GLU:O	1:A:346:PRO:HG2	2.20	0.42
1:B:1229:VAL:CG1	1:B:1231:VAL:CG2	2.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ILE:HG12	1:A:290:TRP:HH2	1.84	0.42
1:B:1185:LEU:HD23	1:B:1185:LEU:C	2.39	0.42
1:B:1359:GLN:OE1	1:B:1359:GLN:HA	2.18	0.42
1:A:203:VAL:CG1	1:A:321:LEU:CD1	2.97	0.42
1:B:1027:ASP:HB2	2:B:89:HOH:O	2.19	0.42
1:A:210:VAL:HB	1:A:223:PHE:HE2	1.85	0.42
1:A:296:VAL:O	1:A:298:GLY:N	2.49	0.42
1:B:1168:GLN:N	2:B:94:HOH:O	2.35	0.42
1:A:9:PRO:HB3	1:A:333:HIS:CE1	2.55	0.42
1:A:40:ARG:HH11	1:A:40:ARG:CB	2.30	0.42
1:B:1290:TRP:CZ2	1:B:1292:GLY:HA3	2.54	0.42
1:A:209:GLN:HE21	1:A:209:GLN:HB3	1.65	0.42
1:A:344:LEU:CD2	1:A:348:LEU:HD12	2.41	0.42
1:A:204:LYS:HG2	1:A:321:LEU:HD22	2.01	0.41
1:A:234:THR:HG1	1:A:237:GLU:HG3	1.83	0.41
1:A:286:SER:OG	1:A:287:PRO:HD2	2.20	0.41
1:A:287:PRO:CB	1:A:314:ARG:HH12	2.22	0.41
1:B:1314:ARG:HA	1:B:1314:ARG:HD3	1.87	0.41
1:A:47:LEU:HD12	1:A:48:ILE:N	2.35	0.41
1:B:1098:SER:O	1:B:1099:ASN:HB3	2.20	0.41
1:A:226:ARG:CD	1:A:327:VAL:HG12	2.50	0.41
1:A:226:ARG:NH1	1:A:226:ARG:CG	2.83	0.41
1:A:228:HIS:HB2	1:A:302:THR:O	2.20	0.41
1:B:1332:PRO:O	1:B:1336:GLU:HB2	2.21	0.41
1:A:226:ARG:HD3	1:A:327:VAL:HG12	2.03	0.41
1:A:351:ALA:O	1:A:353:PRO:HD3	2.21	0.41
1:A:41:LEU:HD23	1:A:41:LEU:HA	1.85	0.41
1:A:52:ARG:HG3	2:A:467:HOH:O	2.20	0.41
1:A:221:ILE:HG12	1:A:222:ARG:H	1.86	0.41
1:B:1081:VAL:HG12	1:B:1120:VAL:CG2	2.43	0.41
1:B:1143:GLN:O	1:B:1144:ARG:HB2	2.20	0.41
1:B:1195:THR:O	1:B:1225:ILE:HG13	2.21	0.41
1:B:1290:TRP:CD2	1:B:1292:GLY:HA3	2.56	0.41
1:A:48:ILE:HD12	1:A:61:ALA:HB2	2.03	0.41
1:A:106:LEU:HB2	1:A:175:PHE:CD1	2.53	0.41
1:A:59:LEU:HD21	1:B:1058:TRP:HB3	2.04	0.40
1:A:78:ARG:HA	1:A:79:PRO:HD3	1.91	0.40
1:A:85:THR:O	1:A:86:VAL:C	2.58	0.40
1:A:313:ALA:HA	2:A:430:HOH:O	2.21	0.40
1:B:1226:ARG:HD2	1:B:1327:VAL:O	2.21	0.40
1:A:231:VAL:HG12	2:A:400:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1074:LEU:HD11	1:B:1105:ASN:HB2	2.03	0.40
1:A:314:ARG:N	1:A:314:ARG:HD3	2.36	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	324/380 (85%)	290 (90%)	29 (9%)	5 (2%)	10	10
1	B	324/380 (85%)	292 (90%)	22 (7%)	10 (3%)	4	2
All	All	648/760 (85%)	582 (90%)	51 (8%)	15 (2%)	6	5

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	PRO
1	A	247	SER
1	B	1178	SER
1	B	1247	SER
1	B	1301	GLY
1	A	209	GLN
1	B	1019	THR
1	B	1109	GLY
1	B	1285	ILE
1	A	287	PRO
1	B	1110	SER
1	B	1179	SER
1	A	297	ARG
1	B	1297	ARG
1	B	1079	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	263/302 (87%)	242 (92%)	21 (8%)	12	15
1	B	263/302 (87%)	244 (93%)	19 (7%)	14	18
All	All	526/604 (87%)	486 (92%)	40 (8%)	13	16

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	8	LEU
1	A	40	ARG
1	A	46	VAL
1	A	70	ARG
1	A	78	ARG
1	A	94	LEU
1	A	103	LEU
1	A	120	VAL
1	A	135	THR
1	A	156	VAL
1	A	157	ARG
1	A	172	PRO
1	A	185	LEU
1	A	204	LYS
1	A	213	LYS
1	A	244	ARG
1	A	289	LEU
1	A	304	LEU
1	A	334	LEU
1	A	352	ILE
1	B	1017	LEU
1	B	1021	GLU
1	B	1024	ARG
1	B	1070	ARG
1	B	1071	LEU
1	B	1106	LEU

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Mol	Chain	Res	Type
1	B	1127	ARG
1	B	1135	THR
1	B	1163	PHE
1	B	1164	PRO
1	B	1208	GLU
1	B	1233	GLU
1	B	1236	ASP
1	B	1289	LEU
1	B	1297	ARG
1	B	1310	THR
1	B	1324	ASP
1	B	1334	LEU
1	B	1343	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	HIS
1	A	124	HIS
1	A	155	HIS
1	A	183	GLN
1	A	209	GLN
1	A	248	HIS
1	A	316	ASN
1	B	1028	HIS
1	B	1099	ASN
1	B	1113	GLN
1	B	1136	GLN
1	B	1209	GLN
1	B	1240	GLN
1	B	1359	GLN

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 monosaccharides 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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.