



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:06 AM UTC

PDB ID : 1M41 / pdb_00001m41
Title : Crystal structure of Escherichia coli alkanesulfonate monooxygenase SsuD at 2.3 Å 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 ⓘ 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

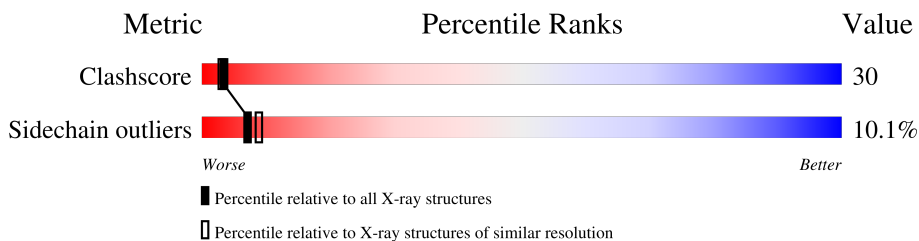
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	190562	6919 (2.30-2.30)
Sidechain outliers	187428	6854 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	380	
1	B	380	

2 Entry composition

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
1	A	328	Total	C	N	O	S	0	0	0
			2549	1628	450	468	3			
1	B	328	Total	C	N	O	S	0	0	0
			2549	1628	450	468	3			

- Molecule 2 is water.

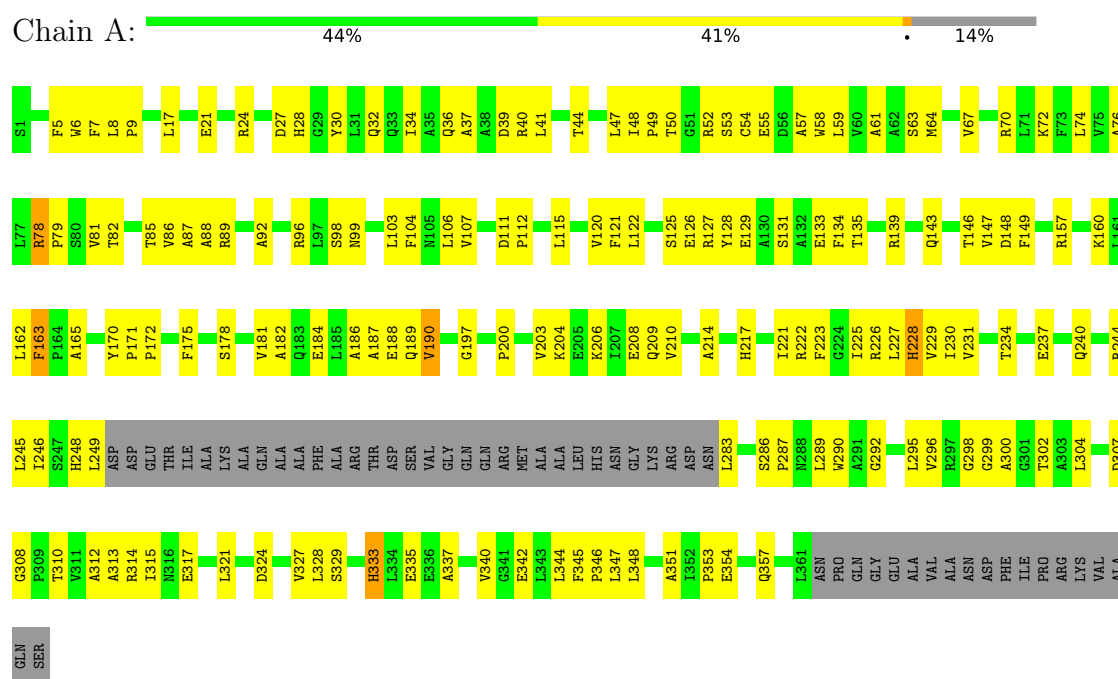
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	144	Total	O	0	0
			144	144		
2	B	166	Total	O	0	0
			166	166		

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. 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



- Molecule 1: FMNH2-dependent alkanesulfonate monooxygenase



GLN	P1309	I1245
SER	T1310	I1246
	V1311	S1247
		H1248
	R1314	L1249
	I1315	ASP
	N1316	ASP
	E1317	GLU
	Y1318	THR
	A1319	ILE
		ALA
	I1323	LYS
	D1324	ALA
	S1325	GLN
	F1326	ALA
	V1327	ALA
	L1328	PHE
		ALA
	Y1331	ARG
	P1332	THR
	H1333	ASP
	L1334	SER
	E1335	VAL
	E1336	GLY
	A1337	GLN
	Y1338	GLN
	R1339	ARG
	V1340	MET
		ALA
	L1343	ALA
	L1344	LEU
		HIS
	V1350	ASN
	A1351	GLY
	I1352	LYS
	P1353	ARG
	E1354	ASP
	I1355	ASN
	P1356	I1283
		E1284
	Q1359	
	P1360	P1287
	L1361	N1288
	ASN	L1289
	PRO	A1291
	GLN	G1292
	GLY	V1293
	GLU	G1294
	ALA	L1295
	VAL	V1296
	ALA	R1297
	ASN	
	ASP	
	PHE	A1300
	ILE	G1301
	PRO	T1302
	ARG	A1303
	LYS	
	VAL	D1307
	ALA	G1308

4 Data and refinement statistics

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 ⓘ

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	0.66	0/2612	1.16	26/3559 (0.7%)
1	B	0.66	0/2612	1.17	24/3559 (0.7%)
All	All	0.66	0/5224	1.17	50/7118 (0.7%)

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	VAL	N-CA-C	8.50	121.06	112.90
1	B	1008	LEU	CA-C-N	8.09	129.96	119.84
1	B	1008	LEU	C-N-CA	8.09	129.96	119.84
1	B	1048	ILE	CA-C-N	7.89	127.84	120.03
1	B	1048	ILE	C-N-CA	7.89	127.84	120.03
1	A	333	HIS	N-CA-C	7.77	122.33	113.01
1	B	1049	PRO	N-CA-C	7.45	122.58	111.41
1	B	1147	VAL	N-CA-C	7.40	118.55	107.75
1	B	1065	ILE	CA-C-N	-7.33	112.25	119.87
1	B	1065	ILE	C-N-CA	-7.33	112.25	119.87
1	A	55	GLU	N-CA-C	-7.23	100.52	110.35
1	B	1055	GLU	N-CA-C	-7.16	100.61	110.35
1	B	1146	THR	N-CA-C	-7.11	98.45	109.76
1	A	49	PRO	N-CA-C	6.80	120.74	111.22
1	A	163	PHE	CA-C-N	6.52	127.05	120.14
1	A	163	PHE	C-N-CA	6.52	127.05	120.14
1	B	1011	HIS	N-CA-C	-6.48	105.53	113.50
1	B	1081	VAL	N-CA-C	6.48	120.25	112.80
1	B	1113	GLN	N-CA-C	-6.46	106.13	112.97
1	B	1355	ILE	N-CA-C	-6.38	103.15	108.63
1	A	354	GLU	CA-C-N	-6.33	118.03	122.59
1	A	354	GLU	C-N-CA	-6.33	118.03	122.59
1	B	1228	HIS	N-CA-C	-6.27	100.08	110.17
1	A	147	VAL	N-CA-C	6.17	117.58	108.45
1	A	317	GLU	N-CA-C	-6.12	104.30	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1057	ALA	N-CA-C	6.09	118.89	111.82
1	A	165	ALA	N-CA-C	-6.06	102.72	110.53
1	A	148	ASP	N-CA-C	-5.98	98.53	108.34
1	B	1060	VAL	CB-CA-C	-5.88	104.20	112.14
1	A	133	GLU	N-CA-C	-5.88	104.56	110.97
1	B	1291	ALA	N-CA-C	-5.83	105.74	112.92
1	A	182	ALA	N-CA-C	5.75	117.35	111.14
1	B	1067	VAL	N-CA-C	5.66	118.43	112.83
1	A	228	HIS	N-CA-C	-5.63	100.50	109.96
1	A	146	THR	N-CA-C	-5.56	101.21	110.17
1	A	357	GLN	CA-C-N	5.51	125.43	119.76
1	A	357	GLN	C-N-CA	5.51	125.43	119.76
1	A	57	ALA	N-CA-C	5.50	117.27	111.28
1	B	1041	LEU	N-CA-C	5.45	119.64	112.89
1	A	78	ARG	CA-C-N	5.44	125.78	119.47
1	A	78	ARG	C-N-CA	5.44	125.78	119.47
1	A	103	LEU	N-CA-C	-5.39	100.88	109.23
1	A	190	VAL	N-CA-C	5.38	116.92	109.45
1	A	357	GLN	N-CA-C	-5.25	103.16	109.83
1	B	1165	ALA	N-CA-C	-5.18	103.77	110.19
1	B	1189	GLN	N-CA-C	5.18	121.83	110.80
1	A	337	ALA	N-CA-C	-5.12	105.82	111.71
1	B	1338	TYR	N-CA-C	-5.11	105.80	112.23
1	B	1037	ALA	N-CA-C	-5.10	105.62	111.07
1	A	178	SER	N-CA-C	-5.01	106.01	111.82

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	2549	0	2526	172	0
1	B	2549	0	2523	142	0
2	A	144	0	0	9	0
2	B	166	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5408	0	5049	303	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 30.

All (303) 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:344:LEU:C	1:A:344:LEU:HD23	2.10	0.77
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:1307:ASP:CG	1:B:1310:THR:HG22	2.12	0.75
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: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:A:44:THR:HA	1:A:353:PRO:CG	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1024:ARG:HH12	1:B:1335:GLU:CD	2.04	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: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:A:344:LEU:HD23	1:A:345:PHE:N	2.12	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:6:TRP:CD1	1:A:7:PHE:H	2.17	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:1020:GLU:H	1:B:1020:GLU:CD	2.07	0.61
1:B:1292:GLY:O	1:B:1295:LEU:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1070:ARG:HD3	2:B:2:HOH:O	2.01	0.61
1:A:287:PRO:O	1:A:314:ARG:NH1	2.35	0.60
1:B:1127:ARG:HG3	1:B:1128:TYR:N	2.15	0.60
1:B:1129:GLU:O	1:B:1133:GLU:HG3	2.01	0.60
1:B:1058:TRP:HZ2	1:B:1077:LEU:HD13	1.67	0.60
1:A:127:ARG:NH1	1:A:127:ARG:HB2	2.17	0.60
1:A:127:ARG:HB2	1:A:127:ARG:HH11	1.66	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:B:1020:GLU:CD	1:B:1020:GLU:N	2.60	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:24:ARG:HH12	1:A:335:GLU:CD	2.13	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: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:1006:TRP:CG	1:B:1007:PHE:H	2.23	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1297:ARG:HG3	1:B:1297:ARG:HH11	1.71	0.55
1:A:28:HIS:CD2	1:A:64:MET:HE1	2.42	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:A:6:TRP:CG	1:A:7:PHE:H	2.26	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:1235:ASN:ND2	1:B:1307:ASP:OD2	2.41	0.54
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:A:286:SER:O	1:A:287:PRO:C	2.52	0.52
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: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:1006:TRP:CD1	1:B:1007:PHE:H	2.28	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:A:287:PRO:C	1:A:314:ARG:HH12	2.19	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:1002:LEU:HB2	1:B:1004:MET:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:344:LEU:C	1:A:344:LEU:CD2	2.83	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
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:B:1178:SER:O	1:B:1179:SER:C	2.55	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: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:B:1185:LEU:HD23	1:B:1185:LEU:C	2.39	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:1178:SER:HA	1:B:1193:TYR:HH	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:50:THR:HG21	1:A:107:VAL:HG21	1.97	0.45
1:A:85:THR:O	1:A:86:VAL:C	2.58	0.45
1:A:8:LEU:HD12	1:A:8:LEU:HA	1.74	0.45
1:A:190:VAL:HG23	1:A:221:ILE:HD11	1.98	0.45
1:A:34:ILE:O	1:A:37:ALA:HB3	2.17	0.45
1:A:63:SER:OG	1:A:64:MET:HE2	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:1150:ASN:O	1:B:1150:ASN:CG	2.58	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:A:79:PRO:HA	1:A:134:PHE:CD1	2.52	0.43
1:B:1187:ALA:HB1	1:B:1213:LYS:C	2.43	0.43
1:A:98:SER:O	1:A:99:ASN:HB3	2.18	0.43
1:A:149:PHE:CD2	1:A:149:PHE:C	2.96	0.43
1:A:299:GLY:HA2	2:A:436:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:TYR:CE1	1:A:34:ILE:HD11	2.53	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:B:1294:GLY:C	1:B:1296:VAL:H	2.25	0.43
1:A:228:HIS:CE1	1:A:329:SER:HG	2.35	0.43
1:B:1139:ARG:C	1:B:1143:GLN:HE21	2.24	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:A:307:ASP:OD1	1:A:310:THR:OG1	2.29	0.43
1:A:308:GLY:C	1:A:347:LEU:CD1	2.92	0.43
1:B:1099:ASN:ND2	1:B:1356:PRO:HG2	2.27	0.43
1:B:1307:ASP:CG	1:B:1310:THR:CG2	2.88	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: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
1:A:246:ILE:HG12	1:A:290:TRP:HH2	1.84	0.42
1:A:229:VAL:HG12	1:A:230:ILE:N	2.33	0.42
1:A:203:VAL:CG1	1:A:321:LEU:CD1	2.97	0.42
1:B:1168:GLN:HA	1:B:1169:PRO:C	2.44	0.42
1:B:1359:GLN:OE1	1:B:1359:GLN:HA	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:171:PRO:O	1:A:172:PRO:C	2.59	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: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:344:LEU:O	1:A:345:PHE:C	2.62	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: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
1:B:1074:LEU:HD11	1:B:1105:ASN:HB2	2.03	0.40
1:B:1316:ASN:O	1:B:1317:GLU:C	2.65	0.40
1:B:1143:GLN:O	1:B:1144:ARG:HB2	2.20	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](#)

There are no protein backbone outliers to report in this entry.

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	B	199/302 (66%)	179 (90%)	20 (10%)	7 9

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1024	ARG
1	B	1103	LEU
1	B	1106	LEU
1	B	1114	GLU
1	B	1127	ARG
1	B	1135	THR
1	B	1152	LYS
1	B	1156	VAL
1	B	1164	PRO
1	B	1208	GLU
1	B	1233	GLU
1	B	1246	ILE
1	B	1289	LEU
1	B	1297	ARG
1	B	1310	THR
1	B	1323	ILE
1	B	1334	LEU
1	B	1343	LEU
1	B	1350	VAL
1	B	1352	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1028	HIS
1	B	1099	ASN
1	B	1113	GLN
1	B	1136	GLN
1	B	1209	GLN
1	B	1240	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.