



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:45 PM UTC

PDB ID : 3JV3 / pdb_00003jv3
Title : Structure of SH3E-DH unit of murine intersectin-1L
Authors : Ahmad, K.F.
Deposited on : 2009-09-15
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

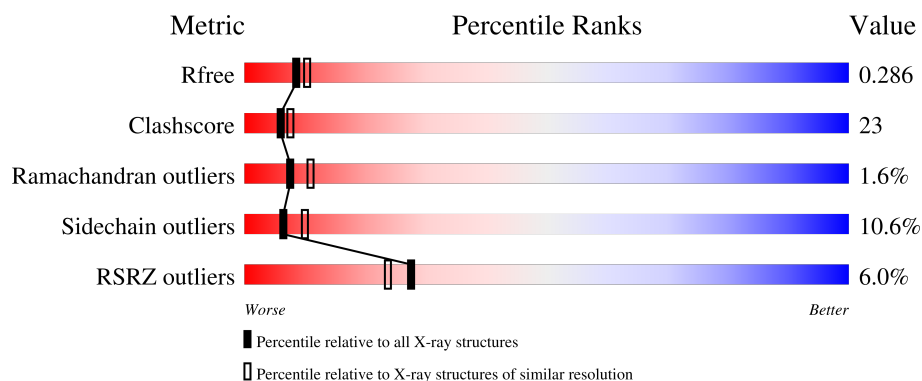
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	283	4% 57% 34% 6% ..
1	B	283	7% 41% 33% 5% 21%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4129 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 Intersectin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	0	0
			2242	1419	382	422	19			
1	B	224	Total	C	N	O	S	0	0	0
			1818	1149	314	338	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9Z0R4
A	0	SER	-	expression tag	UNP Q9Z0R4
B	1149	GLY	-	expression tag	UNP Q9Z0R4
B	1150	SER	-	expression tag	UNP Q9Z0R4

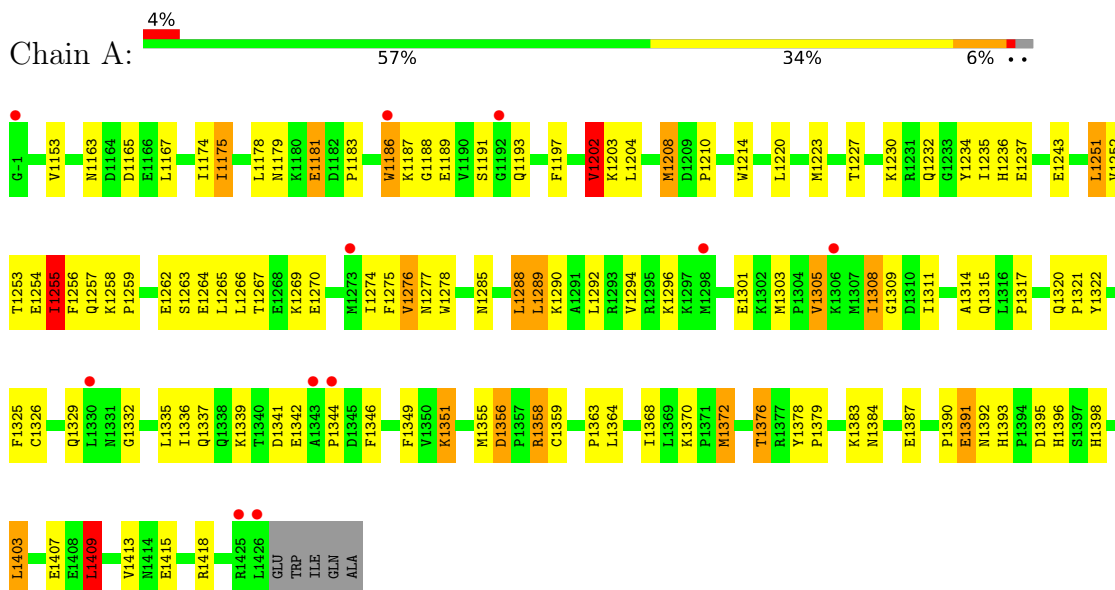
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	42	Total	O	0	0
			42	42		
2	B	27	Total	O	0	0
			27	27		

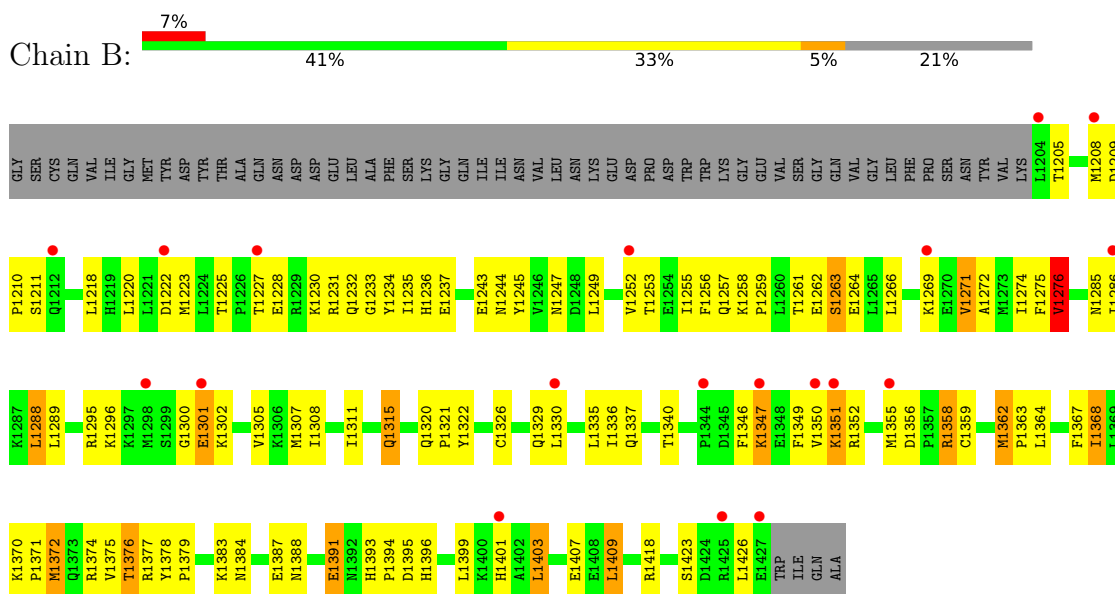
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Intersectin-1



• Molecule 1: Intersectin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	67.04Å 67.04Å 341.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.26 – 2.40 44.26 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.7 (44.26-2.40) 94.8 (44.26-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.67 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.248 , 0.287 0.247 , 0.286	Depositor DCC
R_{free} test set	1787 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	53.5	Xtriage
Anisotropy	0.641	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4129	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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 [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	0.59	0/2286	0.98	6/3086 (0.2%)
1	B	0.54	0/1851	0.96	7/2495 (0.3%)
All	All	0.57	0/4137	0.97	13/5581 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1286	ILE	N-CA-C	-7.16	103.48	110.72
1	A	1202	VAL	N-CA-CB	-6.23	103.80	112.52
1	A	1214	TRP	N-CA-C	6.08	120.86	113.38
1	B	1409	LEU	N-CA-C	-6.05	104.61	111.14
1	A	1356	ASP	N-CA-C	-5.51	101.55	109.48
1	B	1237	GLU	N-CA-C	-5.49	105.21	111.14
1	A	1255	ILE	N-CA-C	5.47	118.25	112.83
1	B	1243	GLU	N-CA-C	-5.47	105.32	111.28
1	A	1409	LEU	N-CA-C	-5.36	105.34	111.07
1	B	1261	THR	N-CA-C	-5.35	106.71	113.18
1	A	1237	GLU	N-CA-C	-5.31	105.49	111.28
1	B	1362	MET	CA-C-N	5.04	124.94	119.85
1	B	1362	MET	C-N-CA	5.04	124.94	119.85

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	2242	0	2258	116	0
1	B	1818	0	1856	86	0
2	A	42	0	0	2	0
2	B	27	0	0	2	0
All	All	4129	0	4114	186	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 23.

All (186) 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:1236:HIS:CE1	1:B:1296:LYS:HE2	2.02	0.94
1:A:1363:PRO:HD3	1:B:1337:GLN:HG2	1.50	0.94
1:A:1418:ARG:HH22	1:B:1384:ASN:HD22	1.09	0.94
1:B:1236:HIS:HE1	1:B:1296:LYS:HE2	1.32	0.93
1:A:1153:VAL:HB	1:A:1202:VAL:HG13	1.49	0.92
1:A:1179:ASN:HD22	1:A:1187:LYS:HE2	1.37	0.90
1:A:1384:ASN:HD22	1:B:1418:ARG:HH22	1.19	0.87
1:A:1255:ILE:HD11	1:A:1359:CYS:SG	2.17	0.85
1:A:1179:ASN:ND2	1:A:1187:LYS:HE2	1.96	0.80
1:A:1418:ARG:HH22	1:B:1384:ASN:ND2	1.78	0.79
1:B:1326:CYS:SG	1:B:1372:MET:HG2	2.22	0.78
1:A:1393:HIS:HD2	1:A:1395:ASP:H	1.30	0.77
1:B:1220:LEU:HD22	1:B:1223:MET:HE2	1.68	0.76
1:B:1205:THR:HA	1:B:1208:MET:HE2	1.66	0.76
1:A:1258:LYS:HB2	1:A:1259:PRO:HD3	1.68	0.75
1:B:1372:MET:O	1:B:1376:THR:HG23	1.86	0.75
1:B:1255:ILE:HD11	1:B:1359:CYS:SG	2.27	0.75
1:B:1393:HIS:HD2	1:B:1395:ASP:H	1.35	0.74
1:A:1276:VAL:HG12	1:A:1277:ASN:H	1.52	0.73
1:B:1232:GLN:O	1:B:1236:HIS:HD2	1.69	0.73
1:A:1153:VAL:HB	1:A:1202:VAL:CG1	2.21	0.71
1:A:1274:ILE:HD13	1:A:1336:ILE:HG12	1.73	0.71
1:B:1383:LYS:O	1:B:1387:GLU:HG3	1.90	0.70
1:A:1236:HIS:CE1	1:A:1296:LYS:HE2	2.27	0.69
1:A:1393:HIS:CD2	1:A:1395:ASP:H	2.10	0.69
1:A:1384:ASN:ND2	1:B:1418:ARG:HH12	1.91	0.69
1:A:1274:ILE:HG23	1:A:1336:ILE:HD11	1.73	0.69
1:A:1351:LYS:HZ2	1:A:1351:LYS:HA	1.58	0.69
1:A:1383:LYS:O	1:A:1387:GLU:HG3	1.94	0.67
1:A:1276:VAL:HG12	1:A:1277:ASN:N	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1337:GLN:NE2	1:A:1337:GLN:HA	2.12	0.65
1:B:1245:TYR:CE2	1:B:1249:LEU:HD11	2.33	0.64
1:A:1337:GLN:HA	1:A:1337:GLN:HE21	1.63	0.64
1:B:1352:ARG:O	1:B:1355:MET:HG2	1.98	0.63
1:B:1231:ARG:HD2	1:B:1388:ASN:O	1.97	0.63
1:B:1263:SER:HB2	1:B:1349:PHE:CE2	2.34	0.63
1:B:1391:GLU:H	1:B:1391:GLU:CD	2.06	0.62
1:B:1266:LEU:HD13	1:B:1271:VAL:HG23	1.81	0.62
1:A:1255:ILE:CD1	1:A:1359:CYS:SG	2.86	0.62
1:B:1285:ASN:ND2	1:B:1322:TYR:OH	2.31	0.62
1:B:1351:LYS:HZ3	1:B:1351:LYS:HB2	1.66	0.60
1:B:1209:ASP:OD2	1:B:1211:SER:OG	2.19	0.60
1:A:1183:PRO:HA	1:A:1186:TRP:HZ3	1.66	0.60
1:B:1295:ARG:HB2	1:B:1311:ILE:HD11	1.84	0.59
1:B:1362:MET:HB3	1:B:1367:PHE:CE1	2.37	0.59
1:B:1256:PHE:CE2	1:B:1364:LEU:HB2	2.37	0.59
1:A:1251:LEU:O	1:A:1255:ILE:HG23	2.02	0.59
1:A:1384:ASN:ND2	1:B:1418:ARG:HH22	1.96	0.58
1:B:1257:GLN:HG3	1:B:1275:PHE:CG	2.39	0.58
1:A:1255:ILE:HG13	1:A:1255:ILE:O	2.02	0.58
1:A:1356:ASP:OD1	1:A:1358:ARG:HD3	2.04	0.58
1:B:1274:ILE:HD13	1:B:1336:ILE:HG12	1.85	0.58
1:A:1263:SER:C	1:A:1265:LEU:H	2.11	0.57
1:B:1274:ILE:HD11	1:B:1335:LEU:HD12	1.87	0.56
1:A:1370:LYS:NZ	2:A:7:HOH:O	2.38	0.56
1:A:1409:LEU:O	1:A:1413:VAL:HG23	2.05	0.56
1:B:1330:LEU:HG	2:B:33:HOH:O	2.04	0.56
1:A:1270:GLU:CD	1:A:1339:LYS:HE2	2.31	0.56
1:B:1266:LEU:CD1	1:B:1271:VAL:HG23	2.36	0.56
1:B:1336:ILE:O	1:B:1340:THR:HG23	2.06	0.56
1:A:1263:SER:HB2	1:A:1349:PHE:CE2	2.41	0.56
1:A:1378:TYR:HB2	1:A:1379:PRO:HD3	1.88	0.55
1:A:1342:GLU:O	1:A:1344:PRO:HD3	2.08	0.54
1:A:1384:ASN:HD21	1:B:1418:ARG:HH12	1.55	0.54
1:A:1418:ARG:NH2	1:B:1384:ASN:ND2	2.54	0.54
1:B:1378:TYR:HB2	1:B:1379:PRO:HD3	1.89	0.54
1:A:1183:PRO:HA	1:A:1186:TRP:CZ3	2.42	0.53
1:A:1285:ASN:ND2	1:A:1322:TYR:OH	2.40	0.53
1:B:1234:TYR:CD1	1:B:1384:ASN:HB3	2.44	0.53
1:A:1232:GLN:O	1:A:1236:HIS:HD2	1.90	0.53
1:A:1288:LEU:HD22	1:A:1292:LEU:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1263:SER:C	1:A:1265:LEU:N	2.65	0.52
1:A:1220:LEU:HD22	1:A:1223:MET:CE	2.39	0.52
1:A:1266:LEU:HB2	1:A:1270:GLU:OE2	2.09	0.52
1:A:1351:LYS:O	1:A:1351:LYS:HD3	2.10	0.52
1:A:1236:HIS:HE1	1:A:1296:LYS:HE2	1.73	0.52
1:A:1153:VAL:HG22	1:A:1175:ILE:HG13	1.92	0.52
1:A:1351:LYS:HA	1:A:1351:LYS:NZ	2.25	0.52
1:A:1390:PRO:HG2	1:A:1393:HIS:HB2	1.91	0.51
1:B:1266:LEU:HD12	1:B:1266:LEU:O	2.10	0.51
1:A:1418:ARG:HB2	1:B:1377:ARG:NE	2.25	0.51
1:A:1263:SER:OG	1:A:1265:LEU:HB2	2.10	0.51
1:B:1210:PRO:HB2	1:B:1233:GLY:HA3	1.92	0.51
1:B:1288:LEU:HA	1:B:1315:GLN:HG2	1.93	0.51
1:A:1266:LEU:HD23	1:A:1346:PHE:CE1	2.45	0.51
1:B:1232:GLN:O	1:B:1236:HIS:CD2	2.58	0.51
1:B:1301:GLU:HG2	1:B:1302:LYS:HG3	1.93	0.51
1:A:1174:ILE:O	1:A:1174:ILE:HG13	2.09	0.50
1:A:1252:VAL:O	1:A:1256:PHE:HB2	2.10	0.50
1:A:1275:PHE:O	1:A:1276:VAL:C	2.54	0.50
1:B:1255:ILE:CD1	1:B:1359:CYS:SG	2.99	0.50
1:B:1252:VAL:O	1:B:1256:PHE:HB2	2.11	0.50
1:A:1220:LEU:HB3	1:A:1223:MET:HE2	1.93	0.50
1:A:1372:MET:O	1:A:1376:THR:HG23	2.12	0.50
1:A:1351:LYS:HB2	1:A:1351:LYS:HZ3	1.77	0.49
1:A:1288:LEU:HA	1:A:1315:GLN:HG2	1.94	0.49
1:B:1274:ILE:HG23	1:B:1336:ILE:HD11	1.94	0.49
1:A:1208:MET:CE	1:B:1426:LEU:HD13	2.42	0.49
1:B:1393:HIS:CD2	1:B:1395:ASP:H	2.24	0.49
1:B:1401:HIS:HB3	2:B:21:HOH:O	2.11	0.49
1:A:1254:GLU:CD	1:A:1358:ARG:HH22	2.21	0.49
1:A:1418:ARG:NH2	1:B:1384:ASN:HD22	1.92	0.49
1:B:1356:ASP:OD1	1:B:1358:ARG:HD3	2.12	0.49
1:A:1274:ILE:CD1	1:A:1336:ILE:HG12	2.41	0.49
1:A:1266:LEU:HD12	1:A:1266:LEU:O	2.12	0.49
1:A:1290:LYS:O	1:A:1294:VAL:HG23	2.13	0.49
1:A:1391:GLU:CD	1:A:1391:GLU:H	2.20	0.49
1:B:1218:LEU:HD12	1:B:1302:LYS:O	2.12	0.49
1:A:1274:ILE:CG2	1:A:1336:ILE:HD11	2.42	0.49
1:A:1418:ARG:HA	1:B:1377:ARG:NH2	2.28	0.48
1:A:1403:LEU:HD22	1:A:1407:GLU:CD	2.37	0.48
1:A:1243:GLU:HA	1:A:1289:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1311:ILE:O	1:A:1315:GLN:HB2	2.14	0.48
1:B:1335:LEU:HD13	1:B:1335:LEU:O	2.14	0.48
1:B:1347:LYS:HB3	1:B:1347:LYS:NZ	2.29	0.48
1:A:1326:CYS:SG	1:A:1372:MET:HG2	2.53	0.48
1:B:1346:PHE:O	1:B:1350:VAL:HG12	2.14	0.48
1:B:1393:HIS:HD2	1:B:1395:ASP:N	2.10	0.47
1:A:1208:MET:HE1	1:B:1426:LEU:HD13	1.96	0.47
1:A:1288:LEU:HD22	1:A:1292:LEU:CD1	2.44	0.47
1:B:1391:GLU:HA	1:B:1396:HIS:CG	2.48	0.47
1:B:1423:SER:HA	1:B:1426:LEU:HD12	1.97	0.47
1:B:1210:PRO:HG2	1:B:1230:LYS:HA	1.96	0.47
1:B:1320:GLN:N	1:B:1321:PRO:CD	2.77	0.47
1:B:1370:LYS:HB2	1:B:1371:PRO:HD3	1.96	0.47
1:A:1384:ASN:HD22	1:B:1418:ARG:NH2	2.00	0.47
1:A:1314:ALA:O	1:A:1317:PRO:HD2	2.15	0.46
1:A:1275:PHE:O	1:A:1278:TRP:HB2	2.14	0.46
1:B:1393:HIS:CD2	1:B:1394:PRO:HD2	2.51	0.46
1:A:1255:ILE:HD12	1:A:1356:ASP:CB	2.45	0.46
1:B:1255:ILE:O	1:B:1255:ILE:HG13	2.15	0.46
1:B:1300:GLY:O	1:B:1301:GLU:C	2.59	0.46
1:B:1403:LEU:HD22	1:B:1407:GLU:HG3	1.96	0.46
1:B:1228:GLU:O	1:B:1228:GLU:HG3	2.17	0.45
1:A:1235:ILE:HD13	1:A:1305:VAL:HG22	1.99	0.45
1:A:1230:LYS:HE3	2:A:28:HOH:O	2.16	0.45
1:B:1245:TYR:CE1	1:B:1374:ARG:HB2	2.51	0.45
1:A:1339:LYS:C	1:A:1341:ASP:H	2.25	0.45
1:A:1210:PRO:HG2	1:A:1230:LYS:HA	1.99	0.44
1:A:1175:ILE:C	1:A:1175:ILE:HD12	2.42	0.44
1:A:1269:LYS:HG3	1:A:1270:GLU:N	2.33	0.44
1:A:1278:TRP:CZ3	1:A:1368:ILE:HD12	2.52	0.44
1:A:1356:ASP:OD2	1:A:1358:ARG:NH1	2.51	0.44
1:B:1205:THR:O	1:B:1208:MET:HB2	2.18	0.44
1:A:1178:LEU:HB2	1:A:1187:LYS:HE3	1.99	0.44
1:A:1234:TYR:CD1	1:A:1384:ASN:HB3	2.54	0.43
1:B:1355:MET:O	1:B:1356:ASP:C	2.60	0.43
1:A:1278:TRP:HZ3	1:A:1368:ILE:HD12	1.82	0.43
1:A:1332:GLY:O	1:A:1336:ILE:HG13	2.19	0.43
1:B:1308:ILE:HG23	1:B:1399:LEU:HD21	2.00	0.43
1:A:1202:VAL:CG1	1:A:1203:LYS:N	2.81	0.43
1:A:1325:PHE:HZ	1:A:1368:ILE:CD1	2.31	0.43
1:B:1258:LYS:HB2	1:B:1259:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1309:GLY:C	1:A:1398:HIS:HB3	2.43	0.43
1:A:1153:VAL:CG2	1:A:1175:ILE:HG13	2.47	0.43
1:A:1153:VAL:HG12	1:A:1204:LEU:HD23	1.99	0.43
1:A:1320:GLN:N	1:A:1321:PRO:CD	2.81	0.43
1:A:1175:ILE:HD11	1:A:1197:PHE:CE2	2.54	0.43
1:A:1337:GLN:HG2	1:B:1363:PRO:HD3	2.00	0.43
1:A:1403:LEU:O	1:A:1407:GLU:HG3	2.19	0.43
1:A:1188:GLY:HA3	1:A:1197:PHE:HE2	1.84	0.43
1:B:1220:LEU:HD22	1:B:1223:MET:CE	2.42	0.43
1:B:1252:VAL:HG21	1:B:1367:PHE:HB3	2.01	0.42
1:B:1383:LYS:HD2	1:B:1403:LEU:HD11	2.00	0.42
1:A:1390:PRO:HB2	1:A:1392:ASN:OD1	2.20	0.42
1:A:1415:GLU:HA	1:A:1415:GLU:OE1	2.19	0.42
1:A:1232:GLN:O	1:A:1236:HIS:CD2	2.71	0.42
1:B:1368:ILE:HD12	1:B:1368:ILE:HA	1.92	0.42
1:B:1275:PHE:O	1:B:1276:VAL:C	2.62	0.42
1:A:1189:GLU:HA	1:A:1193:GLN:O	2.20	0.42
1:B:1231:ARG:O	1:B:1235:ILE:HG13	2.19	0.42
1:A:1276:VAL:CG1	1:A:1277:ASN:H	2.23	0.41
1:A:1255:ILE:HD12	1:A:1356:ASP:HB3	2.02	0.41
1:A:1186:TRP:HB2	1:A:1197:PHE:CZ	2.55	0.41
1:A:1391:GLU:HA	1:A:1396:HIS:CG	2.55	0.41
1:B:1253:THR:HG22	1:B:1258:LYS:HE2	2.03	0.41
1:A:1253:THR:HA	1:A:1257:GLN:HB2	2.02	0.41
1:B:1272:ALA:O	1:B:1276:VAL:HA	2.20	0.41
1:A:1256:PHE:CG	1:A:1364:LEU:HD13	2.55	0.41
1:B:1295:ARG:NH1	1:B:1307:MET:O	2.51	0.41
1:A:1191:SER:O	1:B:1269:LYS:HE3	2.21	0.41
1:A:1269:LYS:HE3	1:A:1269:LYS:HB2	1.84	0.41
1:A:1325:PHE:CD2	1:A:1325:PHE:C	2.98	0.40
1:A:1163:ASN:HB3	1:A:1165:ASP:OD1	2.20	0.40
1:A:1308:ILE:HG23	1:A:1309:GLY:N	2.36	0.40
1:A:1220:LEU:HD22	1:A:1223:MET:SD	2.61	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	276/283 (98%)	259 (94%)	12 (4%)	5 (2%)	6	9
1	B	222/283 (78%)	208 (94%)	11 (5%)	3 (1%)	9	13
All	All	498/566 (88%)	467 (94%)	23 (5%)	8 (2%)	7	11

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1181	GLU
1	B	1301	GLU
1	A	1276	VAL
1	B	1263	SER
1	A	1301	GLU
1	A	1267	THR
1	B	1276	VAL
1	A	1308	ILE

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	255/259 (98%)	230 (90%)	25 (10%)	7	12
1	B	209/259 (81%)	185 (88%)	24 (12%)	5	8
All	All	464/518 (90%)	415 (89%)	49 (11%)	6	10

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1167	LEU
1	A	1175	ILE
1	A	1181	GLU
1	A	1186	TRP
1	A	1202	VAL
1	A	1208	MET
1	A	1227	THR
1	A	1251	LEU
1	A	1255	ILE
1	A	1262	GLU
1	A	1264	GLU
1	A	1288	LEU
1	A	1289	LEU
1	A	1303	MET
1	A	1305	VAL
1	A	1329	GLN
1	A	1335	LEU
1	A	1351	LYS
1	A	1355	MET
1	A	1358	ARG
1	A	1372	MET
1	A	1376	THR
1	A	1391	GLU
1	A	1403	LEU
1	A	1409	LEU
1	B	1222	ASP
1	B	1225	THR
1	B	1227	THR
1	B	1244	ASN
1	B	1247	ASN
1	B	1262	GLU
1	B	1264	GLU
1	B	1271	VAL
1	B	1276	VAL
1	B	1288	LEU
1	B	1289	LEU
1	B	1305	VAL
1	B	1315	GLN
1	B	1329	GLN
1	B	1347	LYS
1	B	1351	LYS
1	B	1358	ARG
1	B	1368	ILE

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Mol	Chain	Res	Type
1	B	1372	MET
1	B	1375	VAL
1	B	1376	THR
1	B	1391	GLU
1	B	1403	LEU
1	B	1409	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1212	GLN
1	A	1213	GLN
1	A	1236	HIS
1	A	1244	ASN
1	A	1247	ASN
1	A	1257	GLN
1	A	1285	ASN
1	A	1315	GLN
1	A	1318	HIS
1	A	1320	GLN
1	A	1329	GLN
1	A	1331	ASN
1	A	1337	GLN
1	A	1384	ASN
1	A	1393	HIS
1	A	1412	GLN
1	B	1212	GLN
1	B	1213	GLN
1	B	1236	HIS
1	B	1257	GLN
1	B	1285	ASN
1	B	1329	GLN
1	B	1337	GLN
1	B	1384	ASN
1	B	1393	HIS
1	B	1414	ASN

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

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	278/283 (98%)	0.39	11 (3%) 42 38	42, 66, 114, 154	0
1	B	224/283 (79%)	0.52	19 (8%) 16 13	41, 74, 128, 152	0
All	All	502/566 (88%)	0.45	30 (5%) 27 24	41, 69, 124, 154	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-1	GLY	5.2
1	A	1306	LYS	3.7
1	A	1330	LEU	3.6
1	A	1192	GLY	3.5
1	A	1298	MET	3.4
1	A	1426	LEU	3.1
1	A	1425	ARG	3.0
1	B	1427	GLU	2.9
1	A	1344	PRO	2.9
1	A	1186	TRP	2.9
1	B	1298	MET	2.9
1	B	1227	THR	2.7
1	A	1273	MET	2.7
1	B	1351	LYS	2.5
1	A	1343	ALA	2.5
1	B	1425	ARG	2.5
1	B	1344	PRO	2.4
1	B	1204	LEU	2.3
1	B	1350	VAL	2.3
1	B	1286	ILE	2.2
1	B	1212	GLN	2.2
1	B	1355	MET	2.2
1	B	1252	VAL	2.2
1	B	1347	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1330	LEU	2.1
1	B	1401	HIS	2.1
1	B	1301	GLU	2.1
1	B	1208	MET	2.1
1	B	1269	LYS	2.0
1	B	1222	ASP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.