



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:38 PM UTC

PDB ID : 4Q58 / pdb_00004q58
Title : Crystal structure of the plectin 1a actin-binding domain/integrin beta 4 fragment complex
Authors : Song, J.-G.; Kostan, J.; Grishkovskaya, I.; Djinovic-Carugo, K.
Deposited on : 2014-04-16
Resolution : 4.00 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

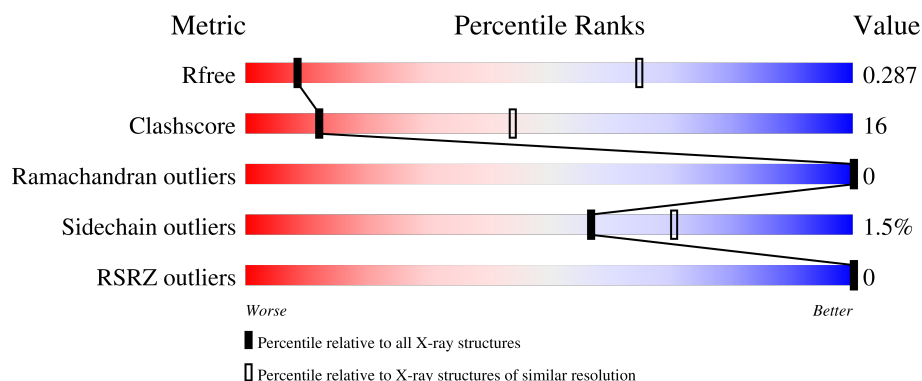
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	226	70% 29% .
1	B	226	73% 25% .
2	C	195	58% 33% . 6%
2	D	195	63% 36% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6619 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 Plectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	20	0	0
			1851	1164	337	344	6			
1	B	223	Total	C	N	O	S	20	0	0
			1830	1154	332	338	6			

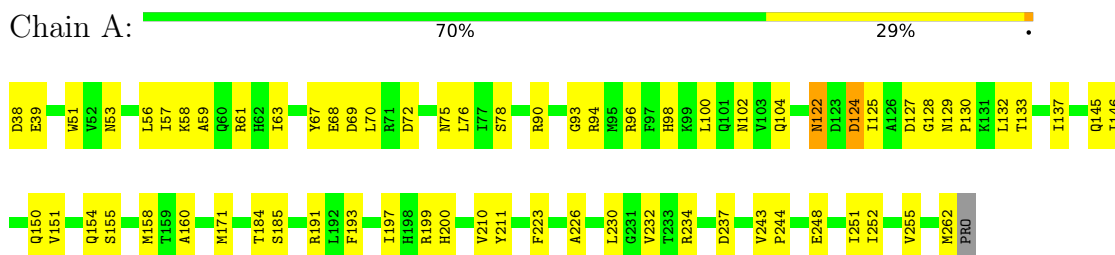
- Molecule 2 is a protein called Integrin beta-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	183	Total	C	N	O	S	0	0	0
			1424	895	246	275	8			
2	D	194	Total	C	N	O	S	0	0	0
			1514	953	264	289	8			

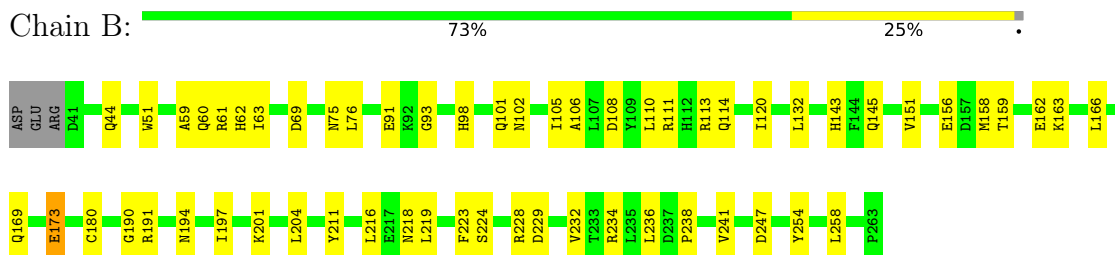
3 Residue-property plots

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.

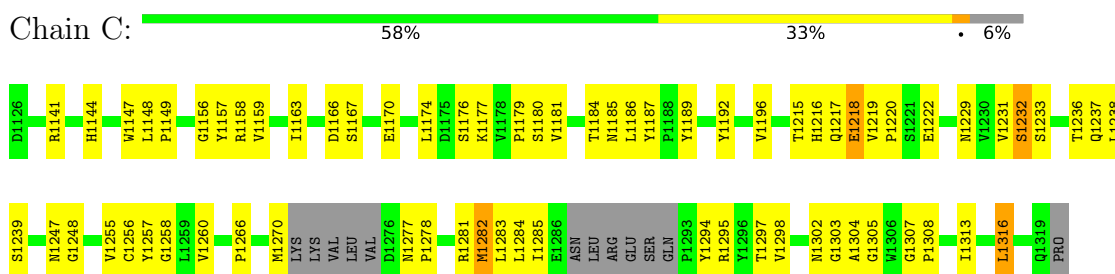
• Molecule 1: Plectin



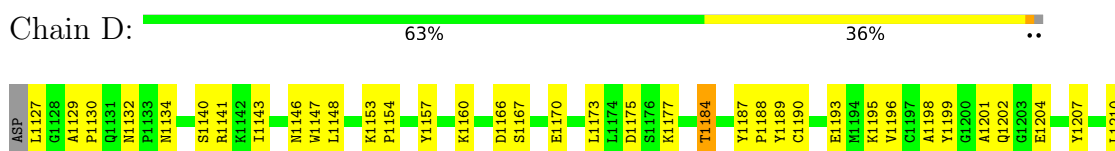
• Molecule 1: Plectin



• Molecule 2: Integrin beta-4



• Molecule 2: Integrin beta-4



T1215	H1216	Q1217	E1218	V1219	P1220	G1224	N1229	V1230	T1236	Q1237	L1238	S1239	V1240	A1241	E1242	P1243	A1244	E1245	T1246	N1247	G1248	Y1253	L1259	D1262	M1270	V1275	R1281	M1282	L1283	L1284	R1295	R1301	N1302	G1303	A1304	G1305	H1306	G1307	E1311	Q1319	P1320
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4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	96.34Å 96.34Å 208.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.93 – 4.00 46.93 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.93-4.00) 98.9 (46.93-4.00)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 4.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.224 , 0.287 0.230 , 0.287	Depositor DCC
R_{free} test set	440 reflections (4.41%)	wwPDB-VP
Wilson B-factor (Å ²)	100.1	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 85.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.079 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6619	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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	0.34	0/1884	0.86	6/2543 (0.2%)
1	B	0.32	0/1864	0.80	2/2518 (0.1%)
2	C	0.36	0/1461	0.83	2/1988 (0.1%)
2	D	0.33	0/1554	0.84	4/2117 (0.2%)
All	All	0.34	0/6763	0.83	14/9166 (0.2%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1282	MET	N-CA-C	10.66	125.58	112.58
1	B	173	GLU	N-CA-C	10.62	122.61	111.14
1	A	122	ASN	N-CA-C	-9.77	100.71	111.36
1	A	125	ILE	N-CA-C	8.59	120.36	111.00
1	A	39	GLU	N-CA-C	-8.37	102.11	111.82
1	A	124	ASP	N-CA-C	8.26	121.10	111.02
1	B	156	GLU	N-CA-C	7.39	121.95	112.34
2	D	1148	LEU	CA-C-N	6.62	124.50	119.66
2	D	1148	LEU	C-N-CA	6.62	124.50	119.66
2	D	1132	ASN	CA-C-N	-5.88	113.91	120.14
2	D	1132	ASN	C-N-CA	-5.88	113.91	120.14
2	C	1232	SER	N-CA-C	5.19	117.56	110.24
1	A	237	ASP	CA-C-N	5.06	125.09	119.32
1	A	237	ASP	C-N-CA	5.06	125.09	119.32

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	1851	0	1859	48	0
1	B	1830	0	1843	44	0
2	C	1424	0	1366	64	0
2	D	1514	0	1474	59	0
All	All	6619	0	6542	204	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 16.

All (204) 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)
2:C:1141:ARG:HG3	2:D:1141:ARG:HD2	1.43	0.99
2:C:1237:GLN:HE21	2:C:1282:MET:CE	1.78	0.96
2:C:1237:GLN:HE21	2:C:1282:MET:HE3	1.35	0.90
1:B:113:ARG:HE	1:B:143:HIS:HE2	1.18	0.90
2:C:1180:SER:O	2:C:1181:VAL:HG13	1.72	0.90
2:C:1236:THR:O	2:C:1284:LEU:HB2	1.72	0.89
1:B:76:LEU:CD2	1:B:106:ALA:HB1	2.03	0.89
1:B:113:ARG:O	1:B:114:GLN:HB2	1.77	0.84
2:C:1231:VAL:HG22	2:C:1232:SER:H	1.47	0.80
1:B:76:LEU:HD22	1:B:106:ALA:CB	2.13	0.79
2:C:1256:CYS:HG	2:C:1297:THR:HG1	1.30	0.75
2:C:1147:TRP:CZ2	2:C:1179:PRO:HA	2.22	0.75
1:A:226:ALA:O	1:A:232:VAL:HG22	1.87	0.75
1:B:76:LEU:CD2	1:B:106:ALA:CB	2.65	0.74
2:C:1184:THR:O	2:C:1185:ASN:OD1	2.05	0.74
2:C:1237:GLN:NE2	2:C:1282:MET:CE	2.49	0.74
2:C:1180:SER:O	2:C:1181:VAL:CG1	2.36	0.74
2:D:1270:MET:SD	2:D:1295:ARG:NH2	2.61	0.73
1:B:201:LYS:HB3	1:B:204:LEU:HD13	1.69	0.73
1:B:223:PHE:HB3	1:B:234:ARG:CG	2.20	0.72
1:B:194:ASN:ND2	1:B:218:ASN:OD1	2.21	0.72
2:C:1231:VAL:HG22	2:C:1232:SER:N	2.06	0.70
2:C:1284:LEU:HD12	2:C:1284:LEU:C	2.16	0.70
2:D:1253:TYR:HB2	2:D:1275:VAL:HG11	1.72	0.70
2:D:1220:PRO:HD3	2:D:1302:ASN:OD1	1.92	0.70
2:C:1256:CYS:SG	2:C:1297:THR:OG1	2.45	0.70
1:A:128:GLY:O	2:D:1281:ARG:NH1	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLN:HB2	1:A:122:ASN:HD21	1.56	0.69
2:C:1255:VAL:HG22	2:C:1298:VAL:HG22	1.74	0.69
2:D:1167:SER:HB2	2:D:1170:GLU:HB2	1.75	0.69
1:B:113:ARG:NE	1:B:143:HIS:NE2	2.36	0.68
1:B:223:PHE:HB3	1:B:234:ARG:HG2	1.75	0.67
2:D:1229:ASN:HB3	2:D:1237:GLN:HB3	1.75	0.67
2:D:1245:GLU:HG2	2:D:1247:ASN:HD21	1.58	0.67
1:B:224:SER:HA	1:B:234:ARG:HH21	1.59	0.66
2:D:1247:ASN:O	2:D:1302:ASN:ND2	2.28	0.66
2:C:1184:THR:O	2:C:1185:ASN:CG	2.39	0.66
2:C:1239:SER:HB2	2:C:1282:MET:SD	2.37	0.65
2:D:1154:PRO:HB3	2:D:1198:ALA:HB1	1.79	0.65
1:B:223:PHE:HB3	1:B:234:ARG:CD	2.28	0.64
2:D:1193:GLU:HB3	2:D:1210:LEU:HD11	1.79	0.64
2:D:1189:TYR:CG	2:D:1248:GLY:HA2	2.33	0.64
2:D:1239:SER:HB2	2:D:1282:MET:HE1	1.81	0.63
1:A:200:HIS:ND1	1:A:262:MET:SD	2.67	0.63
1:A:69:ASP:O	1:A:75:ASN:ND2	2.31	0.62
1:A:226:ALA:HB1	1:A:232:VAL:CG2	2.29	0.62
1:A:124:ASP:CG	1:A:132:LEU:HD13	2.23	0.62
1:A:70:LEU:HD22	1:A:76:LEU:HG	1.80	0.62
2:D:1302:ASN:O	2:D:1304:ALA:N	2.33	0.61
2:D:1175:ASP:OD1	2:D:1199:TYR:OH	2.18	0.61
2:D:1215:THR:HG22	2:D:1216:HIS:N	2.16	0.60
2:C:1238:LEU:HG	2:C:1283:LEU:O	2.01	0.60
1:A:124:ASP:OD2	1:A:132:LEU:HD13	2.01	0.59
1:B:228:ARG:NH1	1:B:229:ASP:OD2	2.35	0.59
2:C:1239:SER:CB	2:C:1282:MET:SD	2.91	0.59
1:B:91:GLU:HG3	1:B:101:GLN:HG3	1.85	0.59
1:A:155:SER:H	1:A:158:MET:HE2	1.67	0.59
1:A:56:LEU:O	1:A:59:ALA:N	2.36	0.58
1:B:69:ASP:O	1:B:75:ASN:ND2	2.35	0.58
1:B:51:TRP:NE1	1:B:145:GLN:OE1	2.32	0.58
1:A:226:ALA:HB1	1:A:232:VAL:HG21	1.86	0.58
1:B:169:GLN:HG3	1:B:180:CYS:HB3	1.86	0.58
2:C:1176:SER:HB2	2:C:1181:VAL:HG12	1.86	0.58
2:D:1219:VAL:HG13	2:D:1307:GLY:HA2	1.86	0.58
1:A:96:ARG:NH1	1:A:127:ASP:OD1	2.34	0.57
2:C:1219:VAL:HG13	2:C:1307:GLY:HA2	1.86	0.57
1:B:120:ILE:HG12	1:B:132:LEU:HD22	1.86	0.57
2:C:1237:GLN:HE21	2:C:1282:MET:HE1	1.66	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1153:LYS:HD3	2:D:1201:ALA:HB3	1.87	0.57
2:D:1134:ASN:OD1	2:D:1146:ASN:ND2	2.37	0.56
2:D:1302:ASN:O	2:D:1303:GLY:C	2.48	0.56
2:C:1233:SER:HA	2:C:1316:LEU:HD22	1.87	0.56
1:B:76:LEU:HD21	1:B:106:ALA:HB1	1.86	0.56
2:C:1220:PRO:HA	2:C:1247:ASN:HD22	1.69	0.56
1:B:158:MET:O	1:B:163:LYS:NZ	2.30	0.56
2:D:1253:TYR:O	2:D:1275:VAL:HG12	2.06	0.56
2:C:1180:SER:C	2:C:1181:VAL:HG13	2.32	0.55
2:C:1258:GLY:HA3	2:C:1270:MET:HB3	1.89	0.55
1:B:169:GLN:O	1:B:173:GLU:HG3	2.07	0.55
1:B:219:LEU:HD21	1:B:241:VAL:HB	1.89	0.55
2:C:1158:ARG:NH2	2:D:1311:GLU:OE1	2.40	0.55
2:C:1222:GLU:HG3	2:C:1308:PRO:HB2	1.88	0.55
2:C:1231:VAL:CG2	2:C:1232:SER:H	2.17	0.55
1:B:113:ARG:NE	1:B:143:HIS:HE2	1.98	0.55
2:C:1233:SER:O	2:C:1316:LEU:HD13	2.07	0.54
2:C:1147:TRP:CE2	2:C:1179:PRO:HA	2.42	0.54
2:D:1224:GLY:HA3	2:D:1241:ALA:HB3	1.88	0.54
1:B:158:MET:HE3	1:B:163:LYS:HG2	1.89	0.54
2:C:1237:GLN:NE2	2:C:1282:MET:HE1	2.19	0.54
2:D:1175:ASP:OD2	2:D:1177:LYS:NZ	2.41	0.53
1:A:63:ILE:HG23	1:A:69:ASP:HB2	1.90	0.53
2:C:1157:TYR:CZ	2:C:1179:PRO:HG3	2.43	0.53
1:A:94:ARG:NH2	2:D:1166:ASP:OD1	2.42	0.53
2:D:1160:LYS:HG2	2:D:1173:LEU:HD22	1.91	0.53
1:A:150:GLN:HA	1:A:154:GLN:NE2	2.24	0.53
1:A:184:THR:OG1	1:A:185:SER:N	2.41	0.52
1:A:59:ALA:O	1:A:61:ARG:N	2.34	0.52
2:D:1199:TYR:HB3	2:D:1204:GLU:HG2	1.91	0.52
2:D:1253:TYR:H	2:D:1275:VAL:CG1	2.22	0.52
2:D:1195:LYS:HG2	2:D:1207:TYR:HB3	1.91	0.51
1:A:56:LEU:O	1:A:58:LYS:N	2.44	0.51
1:B:219:LEU:HD23	1:B:238:PRO:HA	1.93	0.51
2:C:1157:TYR:CE1	2:C:1179:PRO:HG3	2.46	0.51
2:D:1220:PRO:HG3	2:D:1302:ASN:CG	2.34	0.51
2:C:1218:GLU:HG3	2:C:1219:VAL:N	2.26	0.51
1:B:191:ARG:NH2	1:B:211:TYR:O	2.44	0.50
1:A:51:TRP:NE1	1:A:145:GLN:OE1	2.38	0.50
2:C:1176:SER:HB2	2:C:1181:VAL:CG1	2.41	0.50
1:A:56:LEU:O	1:A:57:ILE:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ALA:HA	1:B:60:GLN:CD	2.36	0.50
2:C:1218:GLU:CG	2:D:1184:THR:HG21	2.42	0.50
2:C:1302:ASN:O	2:C:1303:GLY:C	2.56	0.49
2:C:1220:PRO:HD3	2:C:1302:ASN:OD1	2.12	0.49
1:A:171:MET:O	1:A:199:ARG:NH1	2.46	0.49
1:B:93:GLY:HA3	1:B:98:HIS:CD2	2.48	0.49
2:D:1215:THR:CG2	2:D:1216:HIS:N	2.76	0.49
2:C:1149:PRO:HG3	2:C:1179:PRO:HG2	1.95	0.48
1:A:100:LEU:O	1:A:122:ASN:ND2	2.46	0.48
2:C:1187:TYR:O	2:C:1215:THR:HG21	2.12	0.48
1:A:146:ILE:HG22	1:A:160:ALA:HB1	1.94	0.48
2:C:1302:ASN:O	2:C:1304:ALA:N	2.47	0.48
1:A:130:PRO:HG2	2:D:1282:MET:HE3	1.95	0.48
1:B:151:VAL:HG21	1:B:166:LEU:HD23	1.96	0.48
2:D:1302:ASN:O	2:D:1305:GLY:N	2.29	0.48
1:A:93:GLY:HA3	1:A:98:HIS:CG	2.49	0.48
1:A:191:ARG:HH21	1:A:211:TYR:HD1	1.61	0.48
1:B:197:ILE:HD11	1:B:258:LEU:HD11	1.94	0.48
1:B:190:GLY:HA3	1:B:219:LEU:HD12	1.96	0.47
1:A:53:ASN:O	1:A:57:ILE:HG12	2.14	0.47
2:C:1215:THR:OG1	2:C:1216:HIS:N	2.46	0.47
2:C:1258:GLY:O	2:C:1294:TYR:HA	2.14	0.47
2:D:1140:SER:HA	2:D:1216:HIS:HB2	1.96	0.47
1:A:251:ILE:O	1:A:255:VAL:HG23	2.15	0.47
1:B:108:ASP:OD1	1:B:111:ARG:NH2	2.44	0.47
1:A:78:SER:OG	1:A:90:ARG:NH2	2.45	0.47
2:D:1245:GLU:N	2:D:1245:GLU:OE1	2.47	0.47
1:A:129:ASN:HB2	2:D:1241:ALA:HB2	1.96	0.47
1:A:67:TYR:CZ	1:A:130:PRO:HB3	2.51	0.46
2:C:1176:SER:CB	2:C:1181:VAL:CG1	2.94	0.46
2:C:1284:LEU:HD12	2:C:1285:ILE:N	2.30	0.46
2:D:1147:TRP:CZ2	2:D:1196:VAL:HG21	2.50	0.46
2:D:1160:LYS:HG3	2:D:1207:TYR:HE2	1.81	0.46
2:D:1230:VAL:HG21	2:D:1319:GLN:HB3	1.97	0.46
1:B:59:ALA:HA	1:B:60:GLN:CG	2.45	0.46
2:C:1260:VAL:HA	2:C:1266:PRO:HA	1.97	0.46
1:B:159:THR:N	1:B:162:GLU:OE2	2.47	0.46
2:C:1156:GLY:HA3	2:C:1177:LYS:HD3	1.98	0.46
1:B:236:LEU:HD13	1:B:254:TYR:HB2	1.97	0.46
2:C:1163:ILE:O	2:C:1166:ASP:HB2	2.15	0.45
2:D:1187:TYR:HA	2:D:1188:PRO:HD2	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1129:ALA:HA	2:D:1130:PRO:HD3	1.81	0.45
1:A:38:ASP:HB2	2:D:1284:LEU:HD13	1.98	0.45
2:D:1253:TYR:HB2	2:D:1275:VAL:CG1	2.43	0.45
1:B:61:ARG:HD3	1:B:62:HIS:H	1.81	0.45
2:C:1189:TYR:CG	2:C:1248:GLY:HA2	2.51	0.45
1:B:44:GLN:NE2	1:B:247:ASP:OD2	2.37	0.45
2:C:1295:ARG:HA	2:C:1313:ILE:HG12	1.99	0.45
1:A:130:PRO:CG	2:D:1282:MET:HE3	2.47	0.45
2:D:1187:TYR:O	2:D:1190:CYS:HB3	2.17	0.44
1:A:151:VAL:O	1:A:154:GLN:HG3	2.17	0.44
1:A:223:PHE:HB3	1:A:234:ARG:NE	2.32	0.44
1:A:243:VAL:HB	1:A:244:PRO:HD2	1.99	0.44
2:C:1159:VAL:HG22	2:C:1196:VAL:HB	1.99	0.44
2:C:1239:SER:OG	2:C:1282:MET:SD	2.73	0.44
2:D:1236:THR:OG1	2:D:1237:GLN:N	2.49	0.44
1:B:224:SER:CA	1:B:234:ARG:HH21	2.28	0.44
2:C:1186:LEU:HG	2:C:1192:TYR:CZ	2.53	0.44
2:D:1262:ASP:N	2:D:1262:ASP:OD1	2.42	0.44
1:A:72:ASP:O	1:A:102:ASN:ND2	2.38	0.44
1:A:248:GLU:O	1:A:252:ILE:HG13	2.18	0.44
2:C:1277:ASN:HA	2:C:1278:PRO:HD3	1.86	0.44
2:D:1189:TYR:HD1	2:D:1217:GLN:HG2	1.82	0.44
1:B:63:ILE:HG23	1:B:69:ASP:HB2	1.99	0.43
2:C:1148:LEU:HA	2:C:1149:PRO:HD3	1.90	0.43
1:B:113:ARG:HD3	1:B:143:HIS:CE1	2.54	0.43
2:D:1127:LEU:HD21	2:D:1202:GLN:HB3	2.01	0.43
2:C:1302:ASN:O	2:C:1305:GLY:N	2.45	0.42
1:B:101:GLN:O	1:B:105:ILE:HG13	2.18	0.42
1:B:216:LEU:HD22	1:B:216:LEU:H	1.84	0.42
2:C:1231:VAL:CG2	2:C:1232:SER:N	2.74	0.42
2:C:1257:TYR:HA	2:C:1295:ARG:O	2.19	0.42
2:D:1220:PRO:HG3	2:D:1302:ASN:ND2	2.35	0.42
2:D:1301:ARG:HB2	2:D:1306:TRP:CE3	2.54	0.42
1:A:61:ARG:HA	1:A:61:ARG:HD2	1.67	0.42
1:A:96:ARG:HH12	1:A:127:ASP:CG	2.24	0.42
2:C:1156:GLY:HA2	2:C:1177:LYS:HA	2.02	0.42
2:D:1220:PRO:CG	2:D:1302:ASN:CG	2.93	0.41
2:D:1242:GLU:HG3	2:D:1243:PRO:HD2	2.02	0.41
2:C:1141:ARG:CG	2:D:1141:ARG:HD2	2.31	0.41
2:D:1147:TRP:HZ2	2:D:1157:TYR:CD2	2.39	0.41
2:D:1220:PRO:HD3	2:D:1302:ASN:CG	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:PHE:O	1:A:197:ILE:HG12	2.20	0.41
1:A:57:ILE:O	1:A:58:LYS:C	2.64	0.41
1:B:102:ASN:HA	1:B:105:ILE:HD12	2.03	0.41
2:C:1167:SER:O	2:C:1170:GLU:N	2.48	0.41
2:C:1237:GLN:NE2	2:C:1282:MET:HE3	2.17	0.41
1:A:68:GLU:OE2	2:D:1281:ARG:NH2	2.54	0.41
1:A:200:HIS:CD2	1:A:200:HIS:C	3.00	0.40
1:A:56:LEU:HD23	1:A:56:LEU:HA	1.94	0.40
1:A:133:THR:O	1:A:137:ILE:HG12	2.22	0.40
1:B:110:LEU:O	1:B:113:ARG:HB2	2.21	0.40
2:C:1217:GLN:HG2	2:C:1304:ALA:HB2	2.03	0.40
1:A:191:ARG:NH2	1:A:211:TYR:HD1	2.19	0.40
2:D:1259:LEU:H	2:D:1259:LEU:HD22	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	223/226 (99%)	210 (94%)	13 (6%)	0	100	100
1	B	221/226 (98%)	207 (94%)	14 (6%)	0	100	100
2	C	177/195 (91%)	166 (94%)	11 (6%)	0	100	100
2	D	192/195 (98%)	176 (92%)	16 (8%)	0	100	100
All	All	813/842 (97%)	759 (93%)	54 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	207/208 (100%)	205 (99%)	2 (1%)	68	76
1	B	205/208 (99%)	204 (100%)	1 (0%)	81	82
2	C	153/165 (93%)	147 (96%)	6 (4%)	28	51
2	D	164/165 (99%)	162 (99%)	2 (1%)	63	73
All	All	729/746 (98%)	718 (98%)	11 (2%)	57	70

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	210	VAL
1	A	230	LEU
1	B	232	VAL
2	C	1144	HIS
2	C	1174	LEU
2	C	1218	GLU
2	C	1229	ASN
2	C	1281	ARG
2	C	1316	LEU
2	D	1143	ILE
2	D	1184	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	104	GLN
1	A	122	ASN
1	B	104	GLN
1	B	122	ASN
2	C	1237	GLN
2	C	1264	ASN

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 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 [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	225/226 (99%)	-0.18	0 100 100	43, 97, 147, 172	7 (3%)
1	B	223/226 (98%)	-0.33	0 100 100	51, 102, 160, 213	7 (3%)
2	C	183/195 (93%)	-0.02	0 100 100	54, 128, 240, 329	0
2	D	194/195 (99%)	-0.18	0 100 100	57, 125, 192, 230	0
All	All	825/842 (97%)	-0.19	0 100 100	43, 109, 191, 329	14 (1%)

There are no RSRZ outliers to report.

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.