



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:04 AM UTC

PDB ID : 5G1D / pdb_00005g1d
Title : The complex structure of syntenin-1 PDZ domain with c-terminal extension
Authors : Lee, I.; Kim, H.; Yun, J.H.; Lee, W.
Deposited on : 2016-03-25
Resolution : 2.81 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

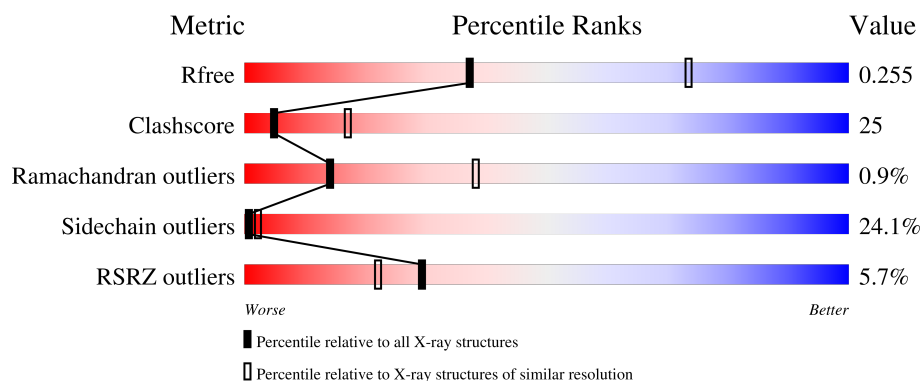
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	201	5% 38% 32% 12% • 16%
1	B	201	4% 46% 27% 9% • 17%
2	C	8	88% 12%
2	D	8	75% 25%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2687 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 SYNTENIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	0	0
			1284	810	230	238	6			
1	B	167	Total	C	N	O	S	0	0	0
			1275	804	228	237	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	GLY	-	expression tag	UNP Q9JI92
A	101	SER	-	expression tag	UNP Q9JI92
A	102	ALA	-	expression tag	UNP Q9JI92
A	103	MET	-	expression tag	UNP Q9JI92
A	104	ALA	-	expression tag	UNP Q9JI92
A	105	ASP	-	expression tag	UNP Q9JI92
A	106	ILE	-	expression tag	UNP Q9JI92
A	107	GLY	-	expression tag	UNP Q9JI92
B	100	GLY	-	expression tag	UNP Q9JI92
B	101	SER	-	expression tag	UNP Q9JI92
B	102	ALA	-	expression tag	UNP Q9JI92
B	103	MET	-	expression tag	UNP Q9JI92
B	104	ALA	-	expression tag	UNP Q9JI92
B	105	ASP	-	expression tag	UNP Q9JI92
B	106	ILE	-	expression tag	UNP Q9JI92
B	107	GLY	-	expression tag	UNP Q9JI92

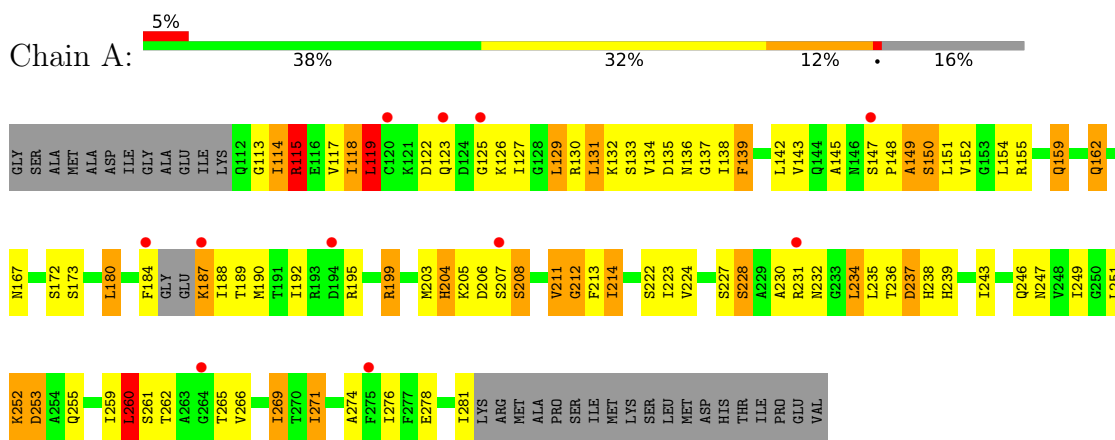
- Molecule 2 is a protein called SYNDECAN-4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	0	0	0
			64	42	9	13			
2	D	8	Total	C	N	O	0	0	0
			64	42	9	13			

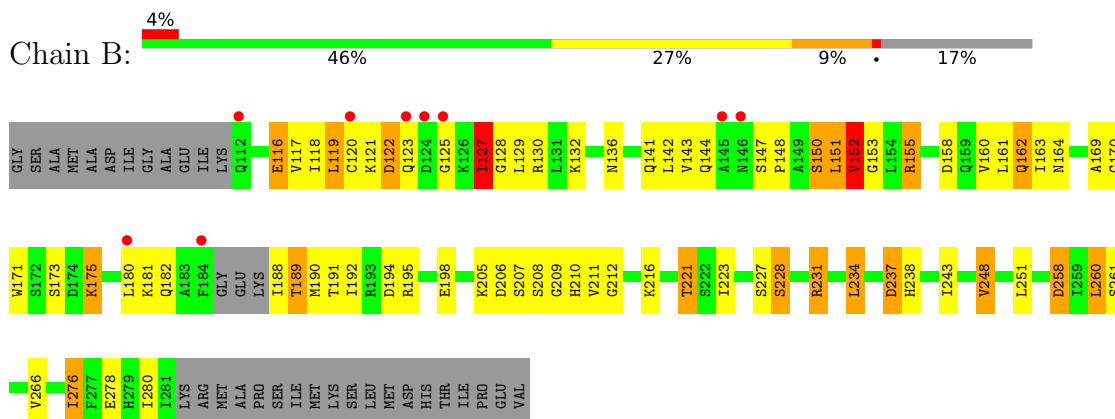
3 Residue-property plots

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.

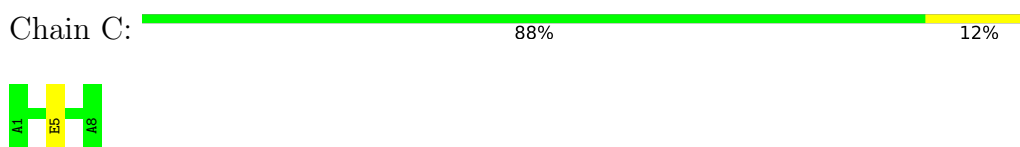
• Molecule 1: SYNTENIN-1



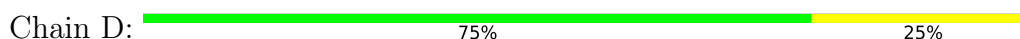
• Molecule 1: SYNTENIN-1



• Molecule 2: SYNDECAN-4



• Molecule 2: SYNDECAN-4





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.53Å 88.53Å 90.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.81 50.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	96.3 (50.00-2.81) 96.6 (50.00-2.81)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.89 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.194 , 0.235 0.221 , 0.255	Depositor DCC
R_{free} test set	667 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.038 for -h,l,k	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	2687	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.71	21/1301 (1.6%)	1.15	9/1751 (0.5%)
1	B	1.78	12/1292 (0.9%)	1.35	3/1740 (0.2%)
2	C	1.68	0/66	1.39	0/90
2	D	1.60	1/66 (1.5%)	1.56	0/90
All	All	1.74	34/2725 (1.2%)	1.27	12/3671 (0.3%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	ILE	C-O	-8.69	1.14	1.24
1	B	152	VAL	CA-CB	-8.65	1.45	1.54
1	A	113	GLY	C-O	-8.11	1.18	1.24
1	A	238	HIS	CG-ND1	-7.99	1.29	1.38
1	B	169	ALA	CA-CB	-7.34	1.41	1.53
1	A	134	VAL	C-O	-6.88	1.16	1.24
1	B	231	ARG	CZ-NH1	-6.73	1.23	1.32
1	B	211	VAL	CA-CB	-6.59	1.46	1.54
1	A	238	HIS	CD2-NE2	-6.39	1.30	1.37
1	A	239	HIS	CG-ND1	-6.28	1.31	1.38
1	A	145	ALA	CA-CB	-6.24	1.43	1.53
1	B	231	ARG	CZ-NH2	-6.24	1.25	1.33
1	A	204	HIS	CG-ND1	-6.22	1.31	1.38
1	A	239	HIS	CD2-NE2	-6.13	1.31	1.37
2	D	1	ALA	N-CA	6.13	1.57	1.46
1	A	117	VAL	C-O	-6.13	1.18	1.24
1	B	171	TRP	CA-C	-6.11	1.44	1.53
1	A	139	PHE	C-O	-5.96	1.16	1.23
1	A	213	PHE	C-O	-5.77	1.16	1.23
1	A	149	ALA	CA-CB	-5.77	1.44	1.53
1	A	132	LYS	C-O	-5.47	1.17	1.23
1	A	204	HIS	CD2-NE2	-5.47	1.31	1.37
1	A	131	LEU	C-O	-5.47	1.17	1.23
1	A	239	HIS	CA-C	-5.32	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	171	TRP	NE1-CE2	-5.31	1.31	1.37
1	B	276	ILE	CA-CB	-5.25	1.47	1.54
1	A	137	GLY	C-O	-5.24	1.15	1.23
1	A	127	ILE	C-O	-5.16	1.18	1.24
1	B	160	VAL	C-O	-5.16	1.18	1.24
1	B	231	ARG	CD-NE	5.14	1.53	1.46
1	A	115	ARG	C-O	-5.09	1.17	1.23
1	B	238	HIS	N-CA	-5.09	1.39	1.45
1	B	175	LYS	C-O	-5.06	1.18	1.24
1	A	172	SER	C-O	-5.04	1.17	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	GLY	N-CA-C	8.93	128.67	115.64
1	A	260	LEU	N-CA-C	8.75	120.59	111.14
1	A	114	ILE	N-CA-C	8.01	119.82	108.36
1	A	253	ASP	N-CA-C	-7.17	103.46	111.71
1	B	153	GLY	N-CA-C	6.61	125.29	115.64
1	A	207	SER	N-CA-C	-6.60	104.09	111.28
1	A	228	SER	N-CA-C	-6.42	103.53	111.75
1	B	151	LEU	N-CA-C	6.39	118.33	111.36
1	A	119	LEU	N-CA-C	5.87	118.33	109.41
1	A	113	GLY	N-CA-C	-5.41	106.40	115.80
1	A	118	ILE	CB-CA-C	-5.28	102.96	110.83
1	B	237	ASP	N-CA-C	5.24	118.66	111.54

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	1284	0	1319	87	0
1	B	1275	0	1306	50	0
2	C	64	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	64	0	56	0	0
All	All	2687	0	2737	137	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 25.

All (137) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:SER:HA	1:A:231:ARG:CD	1.77	1.14
1:A:139:PHE:CE2	1:A:159:GLN:HG3	1.83	1.12
1:A:162:GLN:NE2	1:A:167:ASN:OD1	1.79	1.12
1:A:228:SER:HA	1:A:231:ARG:HD3	1.39	1.01
1:A:139:PHE:CZ	1:A:159:GLN:HG3	2.00	0.95
1:B:119:LEU:HD13	1:B:127:ILE:CD1	1.97	0.94
1:B:258:ASP:N	1:B:258:ASP:OD1	1.98	0.94
1:A:231:ARG:HG3	1:A:232:ASN:ND2	1.83	0.93
1:B:152:VAL:HG23	1:B:152:VAL:O	1.67	0.93
1:A:228:SER:O	1:A:231:ARG:HG2	1.70	0.90
1:A:199:ARG:HH11	1:A:199:ARG:HG3	1.39	0.88
1:B:148:PRO:O	1:B:152:VAL:HG13	1.73	0.88
1:A:228:SER:C	1:A:231:ARG:HG2	2.02	0.85
1:A:119:LEU:N	1:A:119:LEU:HD23	1.93	0.84
1:B:119:LEU:HD13	1:B:127:ILE:HD11	1.56	0.83
1:B:206:ASP:HB3	1:B:208:SER:H	1.43	0.83
1:A:228:SER:HA	1:A:231:ARG:CG	2.10	0.81
1:A:118:ILE:HG12	1:A:189:THR:HG22	1.62	0.81
1:B:136:ASN:HD22	1:B:170:GLY:HA2	1.45	0.81
1:B:206:ASP:HB2	1:B:210:HIS:H	1.46	0.77
1:A:228:SER:O	1:A:231:ARG:CG	2.33	0.76
1:B:122:ASP:O	1:B:125:GLY:N	2.16	0.76
1:A:228:SER:CA	1:A:231:ARG:HG2	2.18	0.73
1:A:162:GLN:HG3	1:A:167:ASN:HA	1.71	0.72
1:A:122:ASP:OD1	1:A:125:GLY:N	2.23	0.72
1:A:155:ARG:HB2	1:A:195:ARG:NH1	2.05	0.71
1:B:119:LEU:HD13	1:B:127:ILE:HD13	1.73	0.71
1:A:203:MET:HB3	1:A:211:VAL:CG2	2.22	0.70
1:A:228:SER:HA	1:A:231:ARG:HG2	1.75	0.69
1:B:155:ARG:HB2	1:B:195:ARG:NH1	2.07	0.69
1:B:148:PRO:O	1:B:152:VAL:CG1	2.41	0.68
1:A:155:ARG:HG3	1:A:195:ARG:NH1	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ARG:CG	1:A:195:ARG:HH12	2.08	0.67
1:A:122:ASP:OD1	1:A:122:ASP:C	2.35	0.67
1:A:203:MET:HB3	1:A:211:VAL:HG22	1.77	0.66
1:A:231:ARG:HG3	1:A:232:ASN:HD22	1.56	0.66
1:A:199:ARG:HG3	1:A:199:ARG:NH1	2.10	0.64
1:A:228:SER:CB	1:A:231:ARG:HE	2.09	0.64
1:A:228:SER:OG	1:A:231:ARG:NE	2.27	0.64
1:B:175:LYS:O	1:B:175:LYS:HG3	1.96	0.63
1:B:243:ILE:HD13	1:B:260:LEU:HD13	1.79	0.63
1:A:147:SER:O	1:A:149:ALA:N	2.32	0.63
1:A:147:SER:O	1:A:150:SER:N	2.30	0.63
1:B:116:GLU:O	1:B:116:GLU:HG3	1.99	0.62
1:A:247:ASN:HD21	1:A:249:ILE:HB	1.65	0.62
1:A:227:SER:O	1:A:230:ALA:N	2.33	0.62
1:A:149:ALA:O	1:A:152:VAL:HG22	2.00	0.61
1:A:204:HIS:HD2	1:A:231:ARG:NH2	1.99	0.60
1:B:119:LEU:HB2	1:B:127:ILE:HD11	1.84	0.60
1:B:206:ASP:HB3	1:B:208:SER:N	2.14	0.59
1:A:155:ARG:HG3	1:A:195:ARG:HH12	1.66	0.58
1:B:119:LEU:HD21	1:B:190:MET:HE3	1.85	0.58
1:B:205:LYS:HB3	1:B:209:GLY:HA2	1.83	0.58
1:B:130:ARG:HB2	1:B:142:LEU:HB3	1.85	0.58
1:A:236:THR:O	1:A:237:ASP:HB2	2.03	0.58
1:A:204:HIS:CD2	1:A:231:ARG:NH2	2.72	0.57
1:A:119:LEU:HD23	1:A:119:LEU:H	1.69	0.57
1:B:155:ARG:HB2	1:B:195:ARG:HH11	1.70	0.57
1:A:119:LEU:N	1:A:119:LEU:CD2	2.66	0.57
1:A:155:ARG:CG	1:A:195:ARG:NH1	2.68	0.57
1:B:158:ASP:OD1	1:B:195:ARG:N	2.34	0.57
1:A:147:SER:O	1:A:148:PRO:C	2.47	0.56
1:A:206:ASP:C	1:A:206:ASP:OD1	2.47	0.56
1:A:228:SER:HA	1:A:231:ARG:NE	2.20	0.56
1:A:212:GLY:O	1:A:224:VAL:HG23	2.06	0.55
1:A:243:ILE:HG21	1:A:260:LEU:CD1	2.36	0.55
1:A:228:SER:O	1:A:232:ASN:ND2	2.29	0.55
1:A:115:ARG:NH2	1:A:152:VAL:O	2.40	0.54
1:B:155:ARG:HD2	1:B:195:ARG:NH1	2.23	0.54
1:A:227:SER:O	1:A:228:SER:C	2.51	0.54
1:A:203:MET:CB	1:A:211:VAL:CG2	2.86	0.54
1:A:139:PHE:CE2	1:A:159:GLN:CG	2.76	0.53
1:B:147:SER:H	1:B:150:SER:HB3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:SER:CA	1:A:231:ARG:CG	2.79	0.52
1:A:135:ASP:O	1:A:136:ASN:HB2	2.10	0.52
1:A:152:VAL:HG23	1:A:154:LEU:HG	1.92	0.52
1:A:155:ARG:HB2	1:A:195:ARG:HH11	1.75	0.52
1:B:276:ILE:O	1:B:280:ILE:HG13	2.10	0.51
1:B:147:SER:H	1:B:150:SER:CB	2.23	0.51
1:A:119:LEU:HB3	1:A:152:VAL:HG11	1.92	0.51
1:A:148:PRO:O	1:A:152:VAL:HG13	2.10	0.51
1:B:258:ASP:HA	1:B:261:SER:HB3	1.93	0.51
1:B:141:GLN:HG3	1:B:280:ILE:O	2.12	0.50
1:A:155:ARG:CB	1:A:195:ARG:NH1	2.73	0.50
1:B:162:GLN:HG2	1:B:191:THR:HB	1.92	0.49
1:B:195:ARG:HD2	1:B:198:GLU:OE1	2.11	0.49
1:B:117:VAL:O	1:B:117:VAL:HG23	2.11	0.49
1:B:119:LEU:CD1	1:B:127:ILE:HD11	2.35	0.49
1:A:204:HIS:HD2	1:A:231:ARG:HH21	1.59	0.49
1:A:234:LEU:HD22	1:A:235:LEU:H	1.78	0.48
1:A:142:LEU:HD12	1:A:143:VAL:N	2.29	0.48
1:B:228:SER:HA	1:B:231:ARG:CG	2.44	0.47
1:B:147:SER:OG	1:B:148:PRO:HD2	2.14	0.47
1:B:164:ASN:N	1:B:189:THR:O	2.38	0.47
1:A:243:ILE:HG23	1:A:269:ILE:HG22	1.97	0.47
1:B:221:THR:HG21	2:C:5:GLU:OE2	2.15	0.47
1:B:234:LEU:HD23	1:B:234:LEU:HA	1.69	0.46
1:B:136:ASN:ND2	1:B:170:GLY:HA2	2.24	0.46
1:B:163:ILE:O	1:B:163:ILE:HG22	2.12	0.45
1:A:212:GLY:HA3	1:A:227:SER:HB2	1.98	0.45
1:A:247:ASN:ND2	1:A:249:ILE:H	2.14	0.45
1:A:142:LEU:HD12	1:A:143:VAL:H	1.82	0.45
1:A:184:PHE:O	1:A:187:LYS:HD3	2.17	0.45
1:A:243:ILE:HG21	1:A:260:LEU:HD13	1.98	0.44
1:B:155:ARG:CB	1:B:195:ARG:HH11	2.29	0.44
1:B:248:VAL:HG22	1:B:251:LEU:HD12	1.99	0.44
1:A:237:ASP:O	1:A:274:ALA:HB2	2.18	0.44
1:A:228:SER:O	1:A:231:ARG:HG3	2.15	0.44
1:A:214:ILE:HB	1:A:222:SER:HB3	1.99	0.44
1:A:252:LYS:O	1:A:253:ASP:C	2.61	0.44
1:B:163:ILE:O	1:B:164:ASN:HB2	2.17	0.44
1:A:180:LEU:HD12	1:A:180:LEU:HA	1.84	0.43
1:A:123:GLN:O	1:A:123:GLN:HG3	2.17	0.43
1:A:269:ILE:HD12	1:A:271:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LEU:HD23	1:A:234:LEU:HA	1.78	0.43
1:A:260:LEU:HD12	1:A:260:LEU:HA	1.89	0.43
1:B:155:ARG:HD2	1:B:195:ARG:HH12	1.81	0.43
1:A:227:SER:H	1:A:230:ALA:HB3	1.84	0.42
1:A:149:ALA:O	1:A:152:VAL:CG2	2.66	0.42
1:A:203:MET:HB2	1:A:211:VAL:HG21	2.00	0.42
1:A:206:ASP:OD1	1:A:208:SER:N	2.53	0.42
1:B:243:ILE:HD13	1:B:260:LEU:CD1	2.47	0.42
1:A:147:SER:C	1:A:149:ALA:N	2.76	0.42
1:A:122:ASP:O	1:A:125:GLY:N	2.42	0.41
1:B:212:GLY:HA3	1:B:227:SER:HB2	2.02	0.41
1:A:205:LYS:NZ	1:A:260:LEU:O	2.44	0.41
1:B:119:LEU:HD12	1:B:188:ILE:HB	2.02	0.41
1:B:117:VAL:O	1:B:117:VAL:CG2	2.68	0.41
1:B:122:ASP:C	1:B:125:GLY:H	2.18	0.41
1:A:243:ILE:HD13	1:A:260:LEU:HD13	2.02	0.41
1:A:129:LEU:HG	1:A:131:LEU:HD21	2.03	0.40
1:A:155:ARG:HB2	1:A:195:ARG:HH12	1.83	0.40
1:A:114:ILE:HG21	1:A:114:ILE:HD13	1.76	0.40
1:B:180:LEU:C	1:B:182:GLN:H	2.29	0.40
1:A:251:LEU:HD23	1:A:251:LEU:HA	1.90	0.40
1:A:129:LEU:HD12	1:A:129:LEU:HA	1.84	0.40
1:B:129:LEU:HD12	1:B:129:LEU:HA	1.86	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	164/201 (82%)	163 (99%)	1 (1%)	0	100	100
1	B	163/201 (81%)	153 (94%)	7 (4%)	3 (2%)	6	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	6/8 (75%)	6 (100%)	0	0	100	100
2	D	6/8 (75%)	6 (100%)	0	0	100	100
All	All	339/418 (81%)	328 (97%)	8 (2%)	3 (1%)	14	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	127	ILE
1	B	181	LYS
1	B	128	GLY

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	142/168 (84%)	105 (74%)	37 (26%)	0	1
1	B	141/168 (84%)	108 (77%)	33 (23%)	1	2
2	C	6/6 (100%)	6 (100%)	0	100	100
2	D	6/6 (100%)	5 (83%)	1 (17%)	2	7
All	All	295/348 (85%)	224 (76%)	71 (24%)	1	2

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	ARG
1	A	119	LEU
1	A	126	LYS
1	A	129	LEU
1	A	130	ARG
1	A	133	SER
1	A	150	SER
1	A	151	LEU
1	A	159	GLN

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Mol	Chain	Res	Type
1	A	162	GLN
1	A	173	SER
1	A	180	LEU
1	A	187	LYS
1	A	188	ILE
1	A	190	MET
1	A	192	ILE
1	A	199	ARG
1	A	208	SER
1	A	211	VAL
1	A	214	ILE
1	A	223	ILE
1	A	234	LEU
1	A	237	ASP
1	A	246	GLN
1	A	252	LYS
1	A	255	GLN
1	A	259	ILE
1	A	260	LEU
1	A	261	SER
1	A	262	THR
1	A	265	THR
1	A	266	VAL
1	A	269	ILE
1	A	271	ILE
1	A	276	ILE
1	A	278	GLU
1	A	281	ILE
1	B	116	GLU
1	B	118	ILE
1	B	119	LEU
1	B	120	CYS
1	B	121	LYS
1	B	122	ASP
1	B	123	GLN
1	B	127	ILE
1	B	132	LYS
1	B	143	VAL
1	B	144	GLN
1	B	150	SER
1	B	151	LEU
1	B	152	VAL

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Mol	Chain	Res	Type
1	B	155	ARG
1	B	161	LEU
1	B	162	GLN
1	B	173	SER
1	B	189	THR
1	B	192	ILE
1	B	194	ASP
1	B	207	SER
1	B	216	LYS
1	B	221	THR
1	B	223	ILE
1	B	228	SER
1	B	234	LEU
1	B	237	ASP
1	B	248	VAL
1	B	258	ASP
1	B	260	LEU
1	B	266	VAL
1	B	278	GLU
2	D	3	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	159	GLN
1	A	204	HIS
1	A	247	ASN
1	B	136	ASN
1	B	141	GLN
1	B	144	GLN
1	B	244	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	168/201 (83%)	0.27	11 (6%) 25 18	9, 31, 58, 88	0
1	B	167/201 (83%)	0.01	9 (5%) 31 23	10, 33, 88, 129	0
2	C	8/8 (100%)	-0.10	0 100 100	22, 33, 38, 42	0
2	D	8/8 (100%)	-0.14	0 100 100	26, 32, 39, 39	0
All	All	351/418 (83%)	0.13	20 (5%) 29 22	9, 32, 69, 129	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	184	PHE	5.4
1	A	184	PHE	4.8
1	B	120	CYS	4.2
1	A	147	SER	4.0
1	B	125	GLY	3.3
1	B	123	GLN	2.9
1	B	124	ASP	2.9
1	B	180	LEU	2.6
1	A	264	GLY	2.6
1	A	187	LYS	2.6
1	A	275	PHE	2.5
1	B	145	ALA	2.5
1	A	231	ARG	2.4
1	A	120	CYS	2.3
1	B	112	GLN	2.3
1	A	194	ASP	2.2
1	A	123	GLN	2.2
1	A	125	GLY	2.1
1	B	146	ASN	2.1
1	A	207	SER	2.1

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.