



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:39 PM UTC

PDB ID : 7ZAS / pdb_00007zas
Title : Crystal structure of cleaved Iripin-4 serpin from tick Ixodes ricinus
Authors : Kascakova, B.; Kuta Smatanova, I.; Chmelar, J.; Prudnikova, T.
Deposited on : 2022-03-22
Resolution : 2.00 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

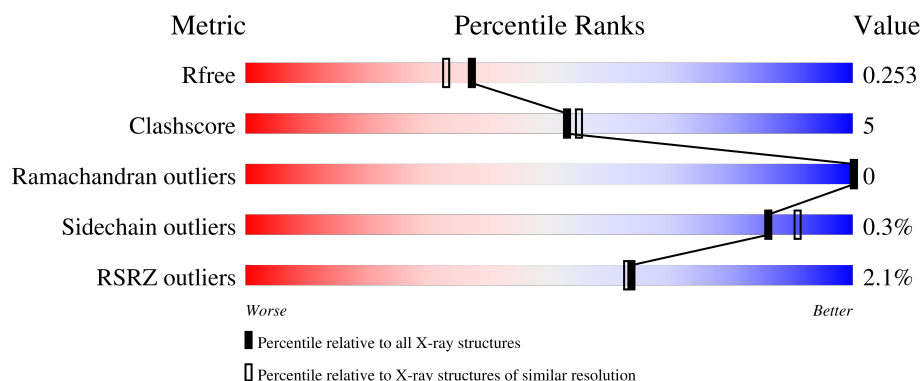
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	341	2% 88% 12%
1	B	341	2% 87% 13%
1	C	341	2% 88% 12%
1	D	341	2% 92% 8%
2	aa	35	6% 77% 14% 9%

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Mol	Chain	Length	Quality of chain
2	bb	35	83% 11% 6%
2	cc	35	6% 94% • •
2	dd	35	77% 14% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13196 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 Iripin-4 serpin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	4	0
			2684	1709	459	510	6			
1	B	341	Total	C	N	O	S	0	4	0
			2685	1710	460	509	6			
1	C	341	Total	C	N	O	S	0	5	0
			2695	1717	461	511	6			
1	D	341	Total	C	N	O	S	0	4	0
			2687	1712	460	509	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	GLN	HIS	variant	UNP A0A0K8RJV9
A	155	GLU	GLY	variant	UNP A0A0K8RJV9
A	307	ASP	GLY	variant	UNP A0A0K8RJV9
B	78	GLN	HIS	variant	UNP A0A0K8RJV9
B	155	GLU	GLY	variant	UNP A0A0K8RJV9
B	307	ASP	GLY	variant	UNP A0A0K8RJV9
C	78	GLN	HIS	variant	UNP A0A0K8RJV9
C	155	GLU	GLY	variant	UNP A0A0K8RJV9
C	307	ASP	GLY	variant	UNP A0A0K8RJV9
D	78	GLN	HIS	variant	UNP A0A0K8RJV9
D	155	GLU	GLY	variant	UNP A0A0K8RJV9
D	307	ASP	GLY	variant	UNP A0A0K8RJV9

- Molecule 2 is a protein called Iripin-4 serpin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	aa	32	Total	C	N	O	0	0	0
			274	179	47	48			
2	bb	33	Total	C	N	O	0	0	0
			281	184	48	49			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	cc	34	Total	C	N	O	0	0	0
			289	190	49	50			
2	dd	32	Total	C	N	O	0	0	0
			274	179	47	48			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		

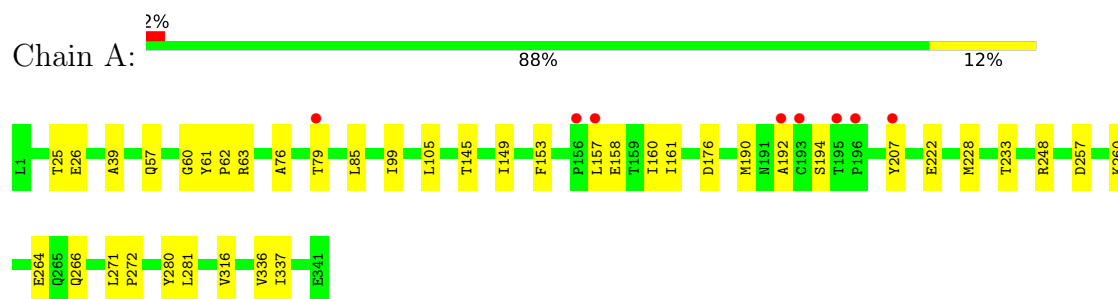
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	287	Total	O	0	14
			300	300		
4	aa	22	Total	O	0	1
			23	23		
4	B	291	Total	O	0	9
			299	299		
4	bb	25	Total	O	0	2
			27	27		
4	C	324	Total	O	0	8
			330	330		
4	cc	31	Total	O	0	0
			31	31		
4	D	272	Total	O	0	18
			288	288		
4	dd	24	Total	O	0	1
			25	25		

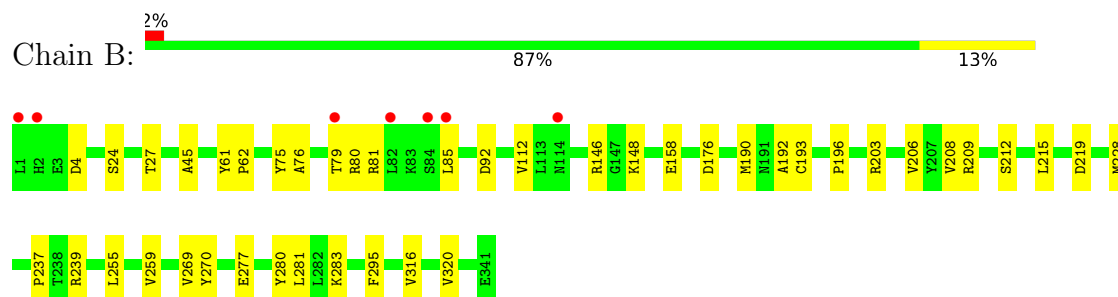
3 Residue-property plots

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.

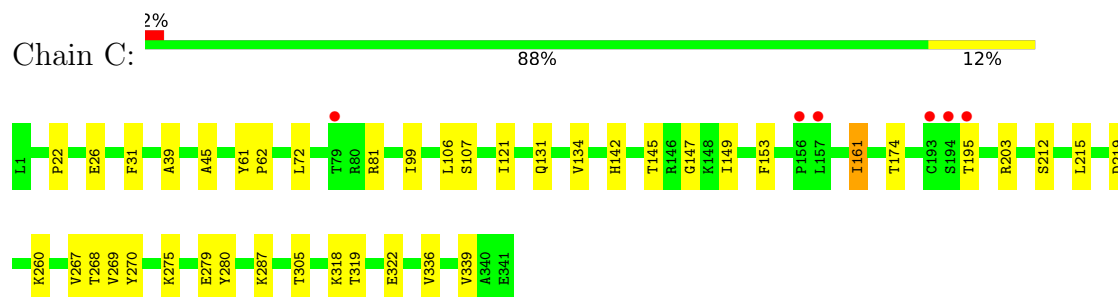
• Molecule 1: Iripin-4 serpin



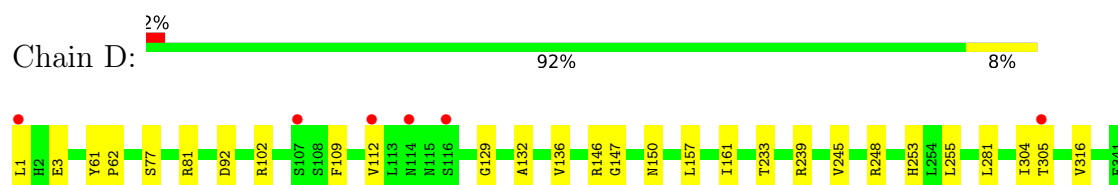
• Molecule 1: Iripin-4 serpin



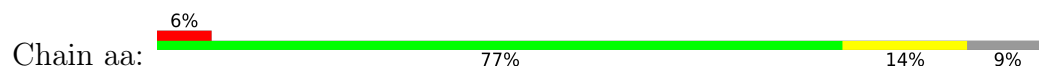
• Molecule 1: Iripin-4 serpin



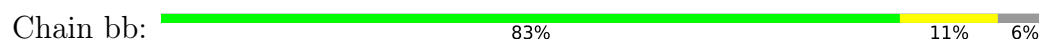
• Molecule 1: Iripin-4 serpin



• Molecule 2: Iripin-4 serpin



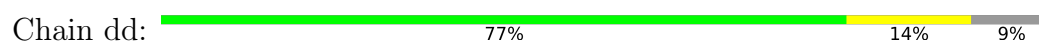
• Molecule 2: Iripin-4 serpin



• Molecule 2: Iripin-4 serpin



• Molecule 2: Iripin-4 serpin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.70Å 138.41Å 80.22Å 90.00° 107.70° 90.00°	Depositor
Resolution (Å)	46.42 – 2.00 46.42 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.42-2.00) 99.5 (46.42-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.187 , 0.250 0.193 , 0.253	Depositor DCC
R_{free} test set	2100 reflections (2.29%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13196	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.37 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3342e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

Bond lengths and bond angles in the following residue types are not validated in this section:
CL

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	1.04	0/2745	1.33	0/3721
1	B	1.03	1/2743 (0.0%)	1.34	0/3719
1	C	1.03	0/2753	1.34	0/3733
1	D	1.01	0/2748	1.31	3/3724 (0.1%)
2	aa	0.97	0/281	1.19	1/378 (0.3%)
2	bb	0.92	0/288	1.13	0/388
2	cc	0.99	0/296	1.15	0/399
2	dd	0.92	0/281	1.11	0/378
All	All	1.02	1/12135 (0.0%)	1.31	4/16440 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	277	GLU	C-O	5.26	1.29	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	253	HIS	CA-CB-CG	-5.90	107.90	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	129	GLY	CA-C-N	5.80	126.55	119.99
1	D	129	GLY	C-N-CA	5.80	126.55	119.99
2	aa	351	VAL	CA-C-O	-5.65	117.71	122.63

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	280	TYR	Peptide
1	B	280	TYR	Peptide
1	C	280	TYR	Peptide

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	2684	0	2705	38	0
1	B	2685	0	2707	30	0
1	C	2695	0	2716	29	0
1	D	2687	0	2713	18	0
2	aa	274	0	265	4	0
2	bb	281	0	274	3	0
2	cc	289	0	285	1	0
2	dd	274	0	265	4	0
3	A	1	0	0	1	0
3	B	1	0	0	1	0
3	C	1	0	0	1	0
3	D	1	0	0	1	0
4	A	300	0	0	3	0
4	B	299	0	0	4	0
4	C	330	0	0	7	0
4	D	288	0	0	3	0
4	aa	23	0	0	3	0
4	bb	27	0	0	0	0
4	cc	31	0	0	1	0
4	dd	25	0	0	1	0
All	All	13196	0	11930	120	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 5.

All (120) 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:157:LEU:HB3	1:A:161:ILE:HD12	1.61	0.81
1:A:79:THR:HB	4:A:716:HOH:O	1.90	0.72
1:D:150:ASN:ND2	4:D:501:HOH:O	2.21	0.72
4:A:686[B]:HOH:O	1:D:248:ARG:NH2	2.26	0.68
1:C:318:LYS:HE2	4:C:520:HOH:O	1.97	0.65
1:A:158:GLU:HG2	1:A:160:ILE:HG12	1.79	0.65
1:B:76:ALA:O	1:B:80:ARG:HG3	1.97	0.65
1:A:158:GLU:CG	1:A:160:ILE:HG12	2.29	0.61
1:D:304:ILE:HG22	1:D:305:THR:HG23	1.82	0.61
1:C:279:GLU:HB3	1:C:318:LYS:HE3	1.82	0.61
1:A:207:TYR:CZ	1:A:266:GLN:HG2	2.36	0.61
1:A:57:GLN:OE1	1:A:63:ARG:NH1	2.34	0.60
1:C:174:THR:HG23	4:C:626:HOH:O	2.01	0.60
1:B:75:TYR:O	1:B:79:THR:HG22	2.01	0.60
3:A:401:CL:CL	3:D:401:CL:CL	2.93	0.59
1:A:176:ASP:CG	1:A:228:MET:HE3	2.28	0.58
1:C:161:ILE:CD1	1:C:339:VAL:HG12	2.33	0.57
1:B:209:ARG:HD2	4:B:720:HOH:O	2.04	0.57
1:B:281:LEU:CD2	1:B:316[B]:VAL:HG22	2.35	0.57
4:C:527:HOH:O	2:cc:375:HIS:HD2	1.88	0.56
1:B:192:ALA:O	1:B:193:CYS:SG	2.63	0.56
1:A:192:ALA:HB2	4:aa:407:HOH:O	2.05	0.56
1:C:81:ARG:HD3	4:C:558:HOH:O	2.05	0.55
1:B:158:GLU:HG3	4:B:671:HOH:O	2.07	0.55
1:D:1:LEU:HB3	1:D:3:GLU:OE2	2.06	0.55
1:C:131:GLN:O	1:C:134:VAL:HG12	2.07	0.54
1:A:248:ARG:HD2	4:A:693:HOH:O	2.07	0.54
2:dd:375:HIS:HE1	4:dd:423:HOH:O	1.90	0.54
1:A:25:THR:HB	1:A:192:ALA:HB3	1.90	0.54
1:B:148:LYS:HB3	1:B:320:VAL:HG21	1.89	0.53
1:C:275:LYS:HG2	1:C:322:GLU:HG3	1.90	0.53
1:D:81:ARG:NH2	4:D:509:HOH:O	2.42	0.52
1:C:39:ALA:HB1	1:C:336:VAL:HG23	1.92	0.52
1:C:267[A]:VAL:HG23	1:C:269:VAL:HG23	1.92	0.52
1:D:239:ARG:HH22	1:D:245:VAL:HG21	1.74	0.52
1:C:22:PRO:HA	4:C:643:HOH:O	2.10	0.51
1:B:4:ASP:HB3	4:B:503:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:LEU:HB2	3:B:401:CL:CL	2.47	0.51
1:A:145:THR:HG21	1:A:149:ILE:HB	1.93	0.51
1:A:260:LYS:HD2	1:B:196:PRO:HD2	1.92	0.51
1:B:206:VAL:HG13	1:B:208:VAL:HG13	1.93	0.51
1:D:109:PHE:O	1:D:112:VAL:HG22	2.11	0.50
1:D:281:LEU:HD23	1:D:316:VAL:HG12	1.93	0.50
1:A:207:TYR:CE2	1:A:266:GLN:HG2	2.47	0.50
1:D:3:GLU:OE2	1:D:77:SER:HB3	2.11	0.50
1:A:161:ILE:HD13	1:A:337:ILE:HG23	1.94	0.50
1:A:157:LEU:HB3	1:A:161:ILE:CD1	2.37	0.49
1:A:158:GLU:HG3	1:A:160:ILE:H	1.77	0.49
1:C:203:ARG:O	1:C:203:ARG:HG3	2.11	0.49
1:C:134:VAL:CG2	1:C:153:PHE:HB2	2.43	0.49
1:A:222:GLU:OE2	2:aa:360:ARG:NH2	2.46	0.48
1:C:212:SER:CB	1:C:219[A]:ASP:OD1	2.62	0.48
1:A:157:LEU:CB	1:A:161:ILE:HD12	2.36	0.48
1:B:176:ASP:CG	1:B:228:MET:HE3	2.38	0.48
1:B:81:ARG:NH1	4:B:503:HOH:O	2.36	0.48
1:B:81:ARG:O	1:B:85:LEU:HG	2.14	0.48
1:C:26:GLU:HG3	4:cc:522:HOH:O	2.13	0.48
1:D:102:ARG:HD3	4:D:701:HOH:O	2.14	0.47
1:A:176:ASP:CB	1:A:228:MET:HE1	2.44	0.47
1:A:257:ASP:HA	1:A:260:LYS:HD3	1.96	0.47
1:B:176:ASP:OD2	1:B:228:MET:HE3	2.14	0.47
1:B:212:SER:OG	1:B:219[A]:ASP:OD1	2.27	0.47
1:A:26:GLU:CG	4:aa:419:HOH:O	2.62	0.47
1:B:190:MET:O	2:bb:354:PRO:HD3	2.15	0.47
1:D:147:GLY:O	1:D:150:ASN:ND2	2.41	0.47
1:A:281:LEU:CD2	1:A:316:VAL:HG12	2.46	0.46
1:B:281:LEU:HD23	1:B:316[B]:VAL:HG22	1.97	0.46
1:A:60:GLY:C	1:A:62:PRO:HD2	2.41	0.46
1:C:106:LEU:HD13	1:C:305:THR:HA	1.97	0.46
1:C:161:ILE:HD13	1:C:339:VAL:HG12	1.97	0.46
1:C:267[A]:VAL:HG23	1:C:269:VAL:CG2	2.46	0.46
1:A:176:ASP:CG	1:A:228:MET:CE	2.89	0.45
1:B:92:ASP:OD2	1:B:146:ARG:NH1	2.37	0.45
1:B:283:LYS:HG3	1:B:295:PHE:CD1	2.51	0.45
1:C:99:ILE:HD12	1:C:121:ILE:HG23	1.98	0.45
1:D:61:TYR:N	1:D:62:PRO:HD2	2.31	0.45
1:A:271:LEU:HD12	1:A:272:PRO:HD2	1.99	0.45
1:D:239:ARG:NH2	1:D:245:VAL:HG21	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:VAL:HG12	1:B:269:VAL:HG23	1.99	0.44
1:B:176:ASP:CG	1:B:228:MET:CE	2.91	0.44
1:B:203:ARG:HG3	1:B:270:TYR:CE1	2.53	0.44
1:A:158:GLU:HG3	1:A:160:ILE:HG12	1.99	0.44
2:bb:353:HIS:HB2	2:bb:354:PRO:CD	2.48	0.44
1:B:45:ALA:HB1	1:B:112:VAL:HG11	2.00	0.43
1:C:161:ILE:HD12	1:C:339:VAL:HG12	1.99	0.43
1:A:190:MET:SD	1:A:194:SER:HA	2.58	0.43
1:C:61:TYR:N	1:C:62:PRO:HD2	2.33	0.43
1:B:206:VAL:CG1	1:B:269:VAL:CG2	2.96	0.43
1:A:61:TYR:N	1:A:62:PRO:HD2	2.34	0.43
1:B:237:PRO:HB2	1:B:239:ARG:O	2.19	0.43
1:A:233:THR:O	2:aa:357:PHE:HA	2.19	0.43
1:C:142:HIS:CE1	1:C:147:GLY:HA2	2.53	0.43
1:C:287:LYS:NZ	4:C:526:HOH:O	2.51	0.42
1:D:92:ASP:OD2	1:D:146:ARG:NH2	2.32	0.42
1:A:99:ILE:HD13	1:A:105:LEU:HD11	2.01	0.42
1:A:153:PHE:CD1	1:A:157:LEU:HD21	2.54	0.42
1:A:281:LEU:HD23	1:A:316:VAL:HG12	2.01	0.42
1:C:215:LEU:HB2	3:C:401:CL:CL	2.57	0.42
1:C:45:ALA:HB2	1:C:72:LEU:HD21	2.01	0.42
1:C:268:THR:HG22	1:C:270:TYR:CE1	2.55	0.42
1:D:233:THR:O	2:dd:357:PHE:HA	2.20	0.42
1:A:190:MET:O	2:aa:354:PRO:HD3	2.19	0.42
1:B:24:SER:H	1:B:27:THR:HB	1.84	0.42
2:bb:357:PHE:CE1	2:bb:371:GLY:HA3	2.55	0.42
2:dd:353:HIS:HB2	2:dd:354:PRO:CD	2.50	0.42
1:A:39:ALA:HB1	1:A:336:VAL:HG23	2.01	0.41
1:D:132:ALA:O	1:D:136:VAL:HG23	2.20	0.41
1:D:255:LEU:HD21	2:dd:358:PHE:CE2	2.54	0.41
1:B:61:TYR:N	1:B:62:PRO:HD2	2.35	0.41
1:D:157:LEU:HB3	1:D:161:ILE:HD12	2.01	0.41
1:A:26:GLU:HG2	4:aa:419:HOH:O	2.20	0.41
1:A:76:ALA:O	1:A:79:THR:HG22	2.21	0.41
1:C:31:PHE:HA	1:C:319:THR:HG21	2.03	0.41
1:A:85:LEU:HD13	2:aa:361:ASN:HD21	1.85	0.41
1:A:176:ASP:HB2	1:A:228:MET:HE1	2.01	0.40
1:B:255:LEU:O	1:B:259:VAL:HG23	2.21	0.40
1:C:39:ALA:HB1	1:C:336:VAL:CG2	2.51	0.40
1:C:145:THR:HG21	1:C:149:ILE:CG1	2.51	0.40
1:B:206:VAL:HG11	1:B:269:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:LYS:HB2	4:C:621:HOH:O	2.20	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	343/341 (101%)	335 (98%)	8 (2%)	0	100	100
1	B	343/341 (101%)	337 (98%)	6 (2%)	0	100	100
1	C	344/341 (101%)	339 (98%)	5 (2%)	0	100	100
1	D	343/341 (101%)	339 (99%)	4 (1%)	0	100	100
2	aa	30/35 (86%)	29 (97%)	1 (3%)	0	100	100
2	bb	31/35 (89%)	30 (97%)	1 (3%)	0	100	100
2	cc	32/35 (91%)	31 (97%)	1 (3%)	0	100	100
2	dd	30/35 (86%)	30 (100%)	0	0	100	100
All	All	1496/1504 (100%)	1470 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	293/289 (101%)	292 (100%)	1 (0%)	86	91
1	B	293/289 (101%)	293 (100%)	0	100	100
1	C	294/289 (102%)	291 (99%)	3 (1%)	68	75
1	D	293/289 (101%)	293 (100%)	0	100	100
2	aa	31/34 (91%)	31 (100%)	0	100	100
2	bb	32/34 (94%)	32 (100%)	0	100	100
2	cc	33/34 (97%)	33 (100%)	0	100	100
2	dd	31/34 (91%)	31 (100%)	0	100	100
All	All	1300/1292 (101%)	1296 (100%)	4 (0%)	86	91

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	264	GLU
1	C	107	SER
1	C	161	ILE
1	C	195	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	88	ASN
1	B	150	ASN
1	C	150	ASN
1	D	19	HIS
1	D	20	ASN
1	D	57	GLN
1	D	88	ASN
1	D	142	HIS
1	D	150	ASN
1	D	261	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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	341/341 (100%)	0.17	8 (2%) 61 60	15, 27, 46, 73	4 (1%)
1	B	341/341 (100%)	0.12	7 (2%) 63 63	9, 25, 46, 79	4 (1%)
1	C	341/341 (100%)	-0.01	6 (1%) 67 67	9, 23, 40, 70	5 (1%)
1	D	341/341 (100%)	0.16	6 (1%) 67 67	13, 27, 47, 69	4 (1%)
2	aa	32/35 (91%)	0.00	2 (6%) 26 24	19, 24, 35, 51	0
2	bb	33/35 (94%)	-0.13	0 100 100	15, 21, 37, 51	0
2	cc	34/35 (97%)	-0.01	2 (5%) 28 27	16, 20, 42, 61	0
2	dd	32/35 (91%)	-0.29	0 100 100	18, 22, 30, 56	0
All	All	1495/1504 (99%)	0.09	31 (2%) 63 63	9, 25, 45, 79	17 (1%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	cc	343	LEU	4.3
1	B	82	LEU	4.0
1	A	192	ALA	3.6
1	B	1	LEU	3.4
1	C	156	PRO	3.3
1	B	79	THR	3.0
1	C	193	CYS	3.0
1	A	156	PRO	2.9
1	A	157	LEU	2.7
1	B	85	LEU	2.7
1	D	112	VAL	2.6
1	D	1	LEU	2.5
1	A	207	TYR	2.5
1	A	79	THR	2.4
1	D	107	SER	2.4
2	cc	344	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	2	HIS	2.3
1	C	157	LEU	2.3
1	A	196	PRO	2.2
1	A	193	CYS	2.2
1	B	84	SER	2.2
1	C	194	SER	2.2
2	aa	358	PHE	2.1
1	D	116	SER	2.1
1	B	114	ASN	2.1
1	A	195	THR	2.1
1	D	114	ASN	2.1
1	C	79	THR	2.1
1	D	305	THR	2.1
1	C	195	THR	2.0
2	aa	346	SER	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	C	401	1/1	0.96	0.07	36,36,36,36	0
3	CL	D	401	1/1	0.96	0.07	41,41,41,41	0
3	CL	A	401	1/1	0.98	0.07	40,40,40,40	0
3	CL	B	401	1/1	0.98	0.04	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.