



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:43 PM UTC

PDB ID : 8U7B / pdb_00008u7b
Title : Crystal structure of Apo form of Short Prokaryotic Argonaute TIR-APAZ (SPARTA) heterodimer
Authors : Kottur, J.; Aggarwal, A.K.
Deposited on : 2023-09-15
Resolution : 2.66 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

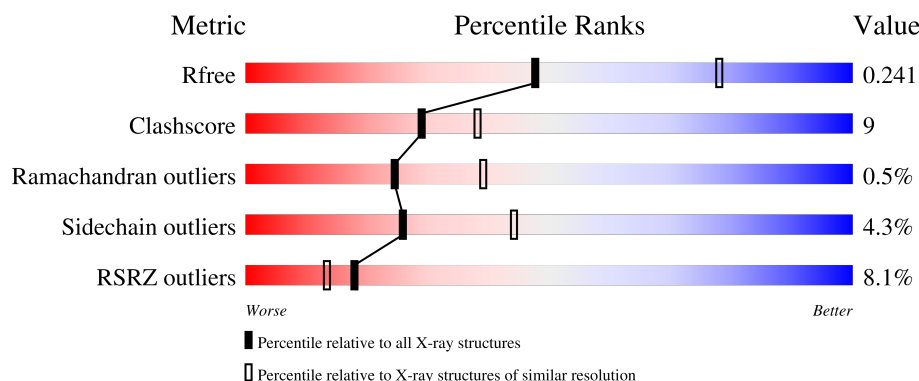
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	B	449	
2	C	507	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7507 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.

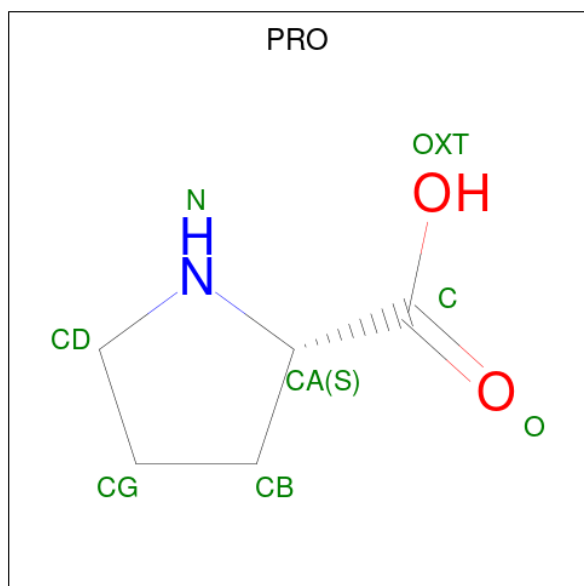
- Molecule 1 is a protein called TIR domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	424	Total	C	N	O	S	1	0	0
			3369	2182	555	622	10			

- Molecule 2 is a protein called Piwi domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	507	Total	C	N	O	S	1	0	0
			3996	2593	665	726	12			

- Molecule 3 is PROLINE (CCD ID: PRO) (formula: $C_5H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			7	5	1	1		
3	B	1	Total	C	N	O	0	0
			7	5	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			7	5	1	1		
3	B	1	Total	C	N	O	0	0
			7	5	1	1		
3	B	1	Total	C	N	O	0	0
			7	5	1	1		
3	C	1	Total	C	N	O	0	0
			7	5	1	1		
3	C	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total	Mn	0	0
			2	2		

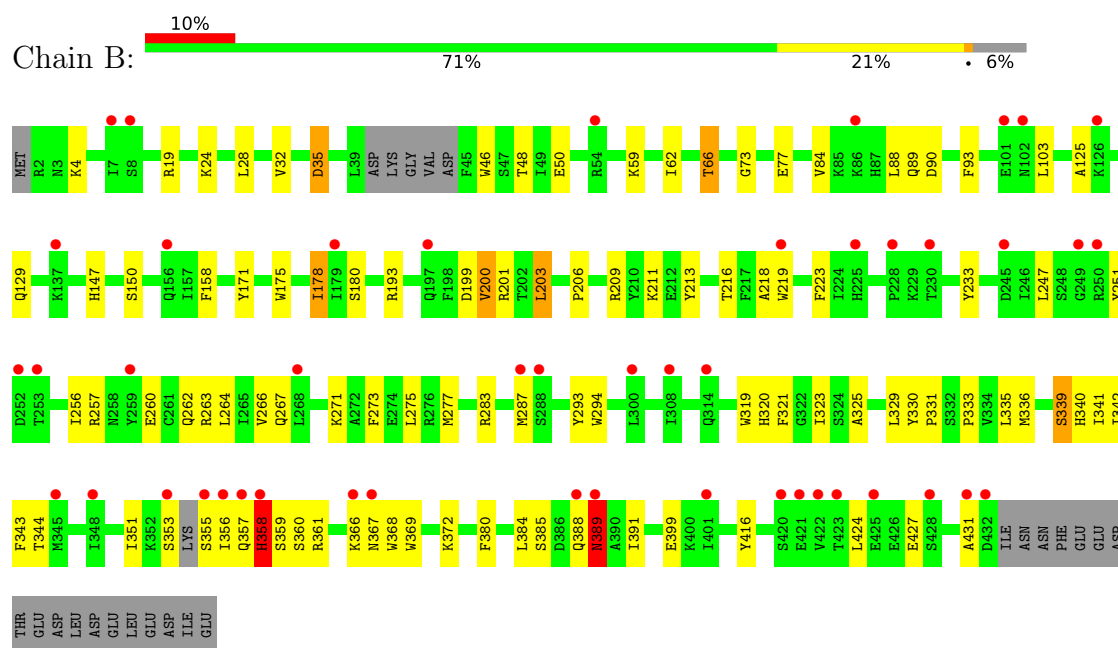
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	37	Total	O	0	0
			37	37		
5	C	54	Total	O	0	0
			54	54		

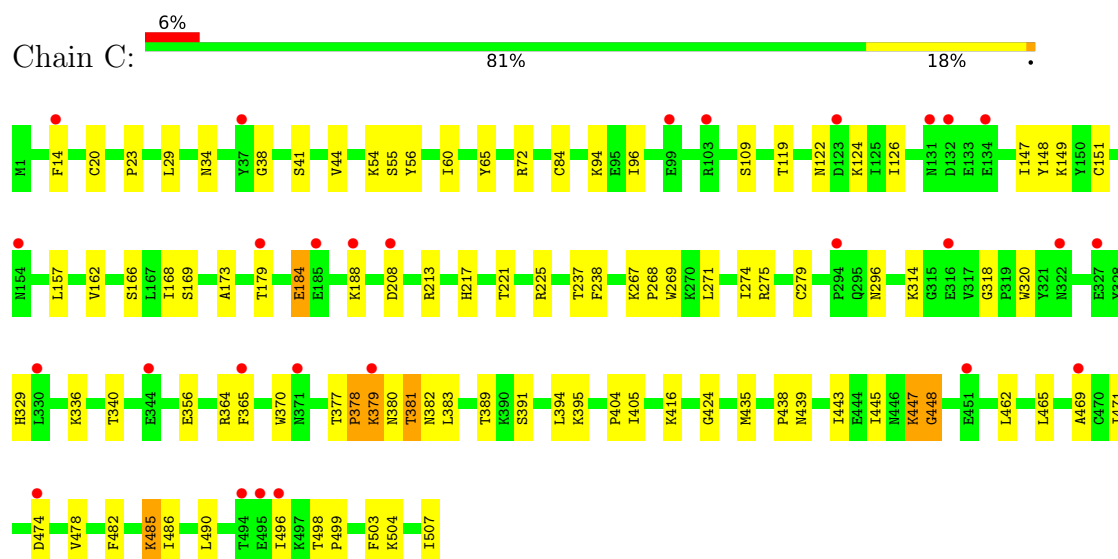
3 Residue-property plots [i](#)

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: TIR domain-containing protein



• Molecule 2: Piwi domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	197.18Å 197.18Å 183.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.71 – 2.66 49.71 – 2.66	Depositor EDS
% Data completeness (in resolution range)	67.6 (49.71-2.66) 67.5 (49.71-2.66)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.20rc3_4406: ???)	Depositor
R, R_{free}	0.179 , 0.239 0.189 , 0.241	Depositor DCC
R_{free} test set	2070 reflections (3.42%)	wwPDB-VP
Wilson B-factor (Å ²)	79.6	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.5	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	0.93	EDS
Total number of atoms	7507	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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](#)

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

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	B	0.30	0/3455	0.42	2/4695 (0.0%)
2	C	0.27	0/4099	0.35	1/5571 (0.0%)
All	All	0.28	0/7554	0.38	3/10266 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	389	ASN	N-CA-C	-6.93	104.13	112.59
1	B	358	HIS	N-CA-C	-5.83	98.38	110.80
2	C	448	GLY	N-CA-C	-5.37	106.66	112.08

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	B	3369	0	3157	71	0
2	C	3996	0	3904	62	0
3	B	35	0	35	2	0
3	C	14	0	14	1	0
4	C	2	0	0	0	0
5	B	37	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	54	0	0	2	0
All	All	7507	0	7110	127	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 9.

All (127) 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:353:SER:C	1:B:355:SER:N	2.22	0.97
1:B:385:SER:HA	1:B:391:ILE:HG12	1.62	0.80
1:B:216:THR:HG22	1:B:218:ALA:H	1.46	0.79
1:B:341:ILE:HB	1:B:361:ARG:HD3	1.64	0.79
1:B:4:LYS:NZ	5:B:601:HOH:O	2.23	0.70
1:B:90:ASP:HB3	1:B:93:PHE:HB2	1.75	0.68
1:B:262:GLN:HB3	1:B:329:LEU:HD21	1.77	0.67
1:B:320:HIS:NE2	1:B:344:THR:OG1	2.28	0.67
2:C:379:LYS:H	2:C:381:THR:HG22	1.64	0.63
1:B:200:VAL:HA	1:B:203:LEU:HD11	1.81	0.62
1:B:35:ASP:N	1:B:35:ASP:OD1	2.33	0.61
2:C:329:HIS:HE1	2:C:364:ARG:O	1.86	0.59
1:B:203:LEU:HD22	1:B:203:LEU:H	1.68	0.59
2:C:34:ASN:HB2	2:C:267:LYS:H	1.68	0.58
2:C:395:LYS:NZ	2:C:439:ASN:OD1	2.37	0.58
1:B:329:LEU:HA	1:B:333:PRO:HA	1.84	0.58
2:C:314:LYS:HD2	2:C:490:LEU:HD22	1.85	0.57
2:C:465:LEU:HB2	2:C:478:VAL:HG21	1.87	0.57
1:B:343:PHE:CE2	1:B:360:SER:HB3	2.40	0.57
1:B:366:LYS:HE2	1:B:431:ALA:HB2	1.87	0.57
2:C:54:LYS:NZ	5:C:701:HOH:O	2.38	0.57
2:C:377:THR:OG1	2:C:383:LEU:HD13	2.03	0.57
1:B:369:TRP:CE2	1:B:424:LEU:HB3	2.40	0.57
1:B:257:ARG:N	1:B:257:ARG:HD2	2.19	0.56
1:B:84:VAL:O	1:B:88:LEU:HD12	2.06	0.56
1:B:199:ASP:C	1:B:201:ARG:H	2.14	0.56
2:C:148:TYR:CD1	2:C:225:ARG:HD3	2.42	0.55
1:B:216:THR:HG21	1:B:223:PHE:HZ	1.71	0.55
1:B:366:LYS:NZ	1:B:367:ASN:OD1	2.40	0.55
1:B:266:VAL:HG13	1:B:329:LEU:HD22	1.89	0.55
2:C:416:LYS:NZ	2:C:448:GLY:O	2.40	0.54
2:C:504:LYS:HA	2:C:507:ILE:HG22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:370:TRP:CD1	2:C:447:LYS:HG2	2.43	0.53
1:B:355:SER:O	1:B:356:ILE:C	2.51	0.53
1:B:361:ARG:HE	3:B:504:PRO:HB2	1.73	0.53
2:C:38:GLY:N	2:C:84:CYS:SG	2.74	0.52
2:C:377:THR:HG22	2:C:381:THR:HG23	1.90	0.52
2:C:378:PRO:HB2	2:C:381:THR:HG22	1.92	0.52
2:C:94:LYS:NZ	5:C:702:HOH:O	2.42	0.52
1:B:73:GLY:O	1:B:77:GLU:HG3	2.11	0.51
1:B:287:MET:HE1	1:B:340:HIS:CD2	2.46	0.51
1:B:263:ARG:O	1:B:267:GLN:HG3	2.11	0.51
2:C:370:TRP:CE2	2:C:447:LYS:HB3	2.46	0.51
2:C:275:ARG:NH2	2:C:356:GLU:OE1	2.45	0.50
2:C:356:GLU:HG2	2:C:382:ASN:HB3	1.93	0.50
1:B:125:ALA:O	1:B:129:GLN:HG3	2.11	0.50
2:C:462:LEU:O	2:C:478:VAL:HG23	2.12	0.50
1:B:171:TYR:CE2	2:C:405:ILE:HG13	2.47	0.49
2:C:122:ASN:O	2:C:126:ILE:HG13	2.12	0.49
1:B:200:VAL:HG21	1:B:209:ARG:HG3	1.93	0.49
1:B:206:PRO:O	1:B:216:THR:HG23	2.12	0.49
2:C:237:THR:HG23	2:C:238:PHE:HD1	1.77	0.49
1:B:271:LYS:O	1:B:275:LEU:HG	2.12	0.49
2:C:14:PHE:CZ	2:C:23:PRO:HA	2.48	0.48
2:C:271:LEU:HG	2:C:465:LEU:HD21	1.95	0.48
1:B:175:TRP:NE1	1:B:336:MET:HG2	2.28	0.48
2:C:237:THR:HG23	2:C:238:PHE:CD1	2.47	0.48
2:C:268:PRO:HB2	2:C:269:TRP:CE3	2.48	0.48
1:B:427:GLU:OE2	2:C:72:ARG:NH2	2.37	0.48
1:B:389:ASN:HD22	1:B:389:ASN:HA	1.48	0.47
2:C:336:LYS:O	2:C:340:THR:OG1	2.25	0.47
2:C:378:PRO:HB2	2:C:381:THR:CG2	2.44	0.47
1:B:325:ALA:HB1	1:B:335:LEU:HD11	1.96	0.47
2:C:416:LYS:HA	2:C:445:ILE:HD12	1.96	0.47
1:B:193:ARG:HD2	1:B:233:TYR:HB2	1.96	0.47
1:B:341:ILE:HD11	1:B:368:TRP:CZ3	2.49	0.47
2:C:119:THR:OG1	2:C:213:ARG:NH2	2.34	0.47
1:B:24:LYS:NZ	2:C:29:LEU:O	2.48	0.47
1:B:416:TYR:OH	2:C:404:PRO:O	2.27	0.47
1:B:294:TRP:HB3	1:B:342:ILE:HD11	1.97	0.47
1:B:319:TRP:HA	1:B:343:PHE:HD1	1.81	0.46
2:C:482:PHE:O	2:C:486:ILE:HG12	2.15	0.46
1:B:59:LYS:HD3	1:B:59:LYS:HA	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:TRP:CE2	2:C:394:LEU:HD13	2.51	0.46
1:B:178:ILE:HG13	1:B:333:PRO:HB2	1.97	0.46
1:B:355:SER:O	1:B:358:HIS:HB2	2.15	0.46
1:B:319:TRP:HB3	1:B:343:PHE:HE1	1.81	0.46
1:B:321:PHE:CZ	1:B:339:SER:HB3	2.51	0.46
2:C:56:TYR:O	2:C:60:ILE:HG12	2.16	0.46
2:C:365:PHE:HB2	2:C:447:LYS:HD2	1.98	0.46
2:C:14:PHE:HE2	2:C:20:CYS:HB3	1.82	0.45
2:C:126:ILE:HD13	2:C:217:HIS:CD2	2.51	0.45
1:B:66:THR:HG23	1:B:103:LEU:HA	1.97	0.45
1:B:211:LYS:C	1:B:213:TYR:H	2.25	0.45
1:B:247:LEU:HD22	1:B:329:LEU:HD12	1.98	0.45
1:B:175:TRP:CD1	1:B:336:MET:HG2	2.52	0.45
1:B:277:MET:HG3	1:B:293:TYR:CD2	2.52	0.45
2:C:469:ALA:HB1	2:C:471:ILE:HG12	1.98	0.45
2:C:96:ILE:HD11	2:C:124:LYS:HG3	1.98	0.44
2:C:147:ILE:O	2:C:151:CYS:HB2	2.17	0.44
2:C:424:GLY:HA2	2:C:438:PRO:HG3	1.98	0.44
1:B:351:ILE:O	1:B:357:GLN:HG3	2.18	0.44
1:B:19:ARG:HG2	1:B:158:PHE:CZ	2.53	0.44
1:B:427:GLU:HB3	2:C:435:MET:HE1	1.99	0.44
2:C:314:LYS:NZ	2:C:496:ILE:O	2.47	0.44
2:C:389:THR:C	2:C:391:SER:H	2.26	0.43
1:B:200:VAL:O	1:B:203:LEU:HD21	2.18	0.43
2:C:379:LYS:C	2:C:381:THR:H	2.27	0.43
1:B:251:TYR:HE2	1:B:256:ILE:HG23	1.83	0.43
2:C:157:LEU:HD23	2:C:162:VAL:HG22	2.01	0.43
2:C:168:ILE:HD13	2:C:173:ALA:HA	2.01	0.43
1:B:341:ILE:HB	1:B:361:ARG:CD	2.40	0.43
1:B:283:ARG:HB2	1:B:294:TRP:CE2	2.54	0.43
1:B:219:TRP:CZ3	1:B:399:GLU:HG2	2.54	0.42
2:C:485:LYS:HD2	2:C:485:LYS:HA	1.72	0.42
1:B:199:ASP:C	1:B:201:ARG:N	2.77	0.42
1:B:323:ILE:HD13	1:B:380:PHE:CD1	2.55	0.42
1:B:424:LEU:HD22	1:B:424:LEU:H	1.84	0.42
1:B:147:HIS:NE2	3:C:603:PRO:HG3	2.35	0.42
2:C:274:ILE:HA	2:C:274:ILE:HD12	1.79	0.42
2:C:377:THR:HG22	2:C:381:THR:CG2	2.51	0.41
2:C:462:LEU:HD23	2:C:462:LEU:HA	1.88	0.41
1:B:28:LEU:HD23	1:B:28:LEU:HA	1.92	0.41
1:B:46:TRP:NE1	1:B:50:GLU:OE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:14:PHE:HZ	2:C:23:PRO:HA	1.86	0.41
2:C:54:LYS:HG3	2:C:55:SER:N	2.35	0.41
1:B:260:GLU:O	1:B:264:LEU:HD22	2.20	0.41
3:B:505:PRO:HD2	2:C:65:TYR:CE2	2.56	0.41
2:C:184:GLU:O	2:C:188:LYS:HG2	2.20	0.41
1:B:319:TRP:HB3	1:B:343:PHE:CE1	2.56	0.40
1:B:273:PHE:CZ	1:B:277:MET:HE3	2.56	0.40
1:B:330:TYR:CD1	1:B:331:PRO:HA	2.57	0.40
2:C:208:ASP:OD1	2:C:485:LYS:NZ	2.47	0.40
2:C:498:THR:HA	2:C:499:PRO:HD3	1.95	0.40
1:B:358:HIS:O	1:B:359:SER:C	2.64	0.40
2:C:94:LYS:HB3	2:C:94:LYS:HE3	1.64	0.40
2:C:318:GLY:HA3	2:C:320:TRP:CZ2	2.56	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	B	418/449 (93%)	390 (93%)	25 (6%)	3 (1%)	18	30
2	C	505/507 (100%)	472 (94%)	31 (6%)	2 (0%)	30	45
All	All	923/956 (96%)	862 (93%)	56 (6%)	5 (0%)	24	39

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	388	GLN
1	B	200	VAL
1	B	358	HIS
2	C	378	PRO
2	C	379	LYS

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	B	345/414 (83%)	330 (96%)	15 (4%)	26	44
2	C	413/446 (93%)	395 (96%)	18 (4%)	25	43
All	All	758/860 (88%)	725 (96%)	33 (4%)	26	43

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	32	VAL
1	B	35	ASP
1	B	48	THR
1	B	62	ILE
1	B	66	THR
1	B	89	GLN
1	B	150	SER
1	B	178	ILE
1	B	180	SER
1	B	203	LEU
1	B	339	SER
1	B	358	HIS
1	B	372	LYS
1	B	384	LEU
1	B	389	ASN
2	C	41	SER
2	C	44	VAL
2	C	109	SER
2	C	149	LYS
2	C	166	SER
2	C	169	SER
2	C	179	THR
2	C	184	GLU
2	C	221	THR
2	C	279	CYS
2	C	296	ASN
2	C	380	ASN

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Mol	Chain	Res	Type
2	C	381	THR
2	C	443	ILE
2	C	447	LYS
2	C	474	ASP
2	C	485	LYS
2	C	503	PHE

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	116	ASN
1	B	340	HIS
1	B	389	ASN
2	C	207	HIS
2	C	329	HIS
2	C	341	GLN

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](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PRO	B	505	-	6,7,8	0.63	0	7,8,10	1.26	1 (14%)
3	PRO	B	504	-	6,7,8	0.61	0	7,8,10	1.27	1 (14%)
3	PRO	C	604	-	6,7,8	0.84	0	7,8,10	1.14	0
3	PRO	B	501	-	6,7,8	0.61	0	7,8,10	1.32	1 (14%)
3	PRO	C	603	-	6,7,8	0.61	0	7,8,10	1.21	0
3	PRO	B	503	-	6,7,8	0.61	0	7,8,10	1.29	1 (14%)
3	PRO	B	502	-	6,7,8	0.59	0	7,8,10	1.36	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PRO	B	505	-	-	0/0/9/11	0/1/1/1
3	PRO	B	504	-	-	0/0/9/11	0/1/1/1
3	PRO	C	604	-	-	0/0/9/11	0/1/1/1
3	PRO	B	501	-	-	0/0/9/11	0/1/1/1
3	PRO	C	603	-	-	0/0/9/11	0/1/1/1
3	PRO	B	503	-	-	0/0/9/11	0/1/1/1
3	PRO	B	502	-	-	0/0/9/11	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	PRO	O-C-CA	-2.31	118.83	124.77
3	B	503	PRO	O-C-CA	-2.26	118.95	124.77
3	B	504	PRO	O-C-CA	-2.10	119.38	124.77
3	B	505	PRO	O-C-CA	-2.10	119.38	124.77
3	B	501	PRO	O-C-CA	-2.05	119.50	124.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	505	PRO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	504	PRO	1	0
3	C	603	PRO	1	0

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	B	424/449 (94%)	0.52	47 (11%) 10 8	32, 78, 111, 162	1 (0%)
2	C	507/507 (100%)	0.23	28 (5%) 30 24	28, 59, 100, 144	5 (0%)
All	All	931/956 (97%)	0.36	75 (8%) 18 13	28, 68, 108, 162	6 (0%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	37	TYR	7.3
1	B	432	ASP	6.1
2	C	494	THR	5.8
1	B	137	LYS	5.1
1	B	86	LYS	4.7
1	B	420	SER	4.6
1	B	197	GLN	4.6
1	B	249	GLY	4.5
2	C	134	GLU	4.4
1	B	353	SER	4.1
1	B	421	GLU	4.0
1	B	225	HIS	4.0
1	B	252	ASP	3.9
2	C	185	GLU	3.8
1	B	422	VAL	3.7
2	C	379	LYS	3.6
1	B	268	LEU	3.5
2	C	495	GLU	3.5
1	B	355	SER	3.4
2	C	496	ILE	3.4
2	C	179	THR	3.4
2	C	344	GLU	3.3
2	C	316	GLU	3.2
1	B	431	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	367	ASN	3.2
2	C	103	ARG	3.2
2	C	131	ASN	3.2
2	C	132	ASP	3.2
1	B	8	SER	3.2
2	C	365	PHE	3.1
1	B	389	ASN	3.0
2	C	451	GLU	3.0
1	B	428	SER	2.9
1	B	308	ILE	2.9
1	B	250	ARG	2.9
1	B	101	GLU	2.9
1	B	102	ASN	2.7
1	B	358	HIS	2.7
2	C	371	ASN	2.7
2	C	99	GLU	2.7
1	B	348	ILE	2.7
1	B	366	LYS	2.7
2	C	123	ASP	2.5
1	B	425	GLU	2.5
1	B	357	GLN	2.5
1	B	345	MET	2.5
2	C	208	ASP	2.5
2	C	14	PHE	2.5
2	C	330	LEU	2.4
1	B	300	LEU	2.4
1	B	219	TRP	2.4
1	B	388	GLN	2.4
1	B	156	GLN	2.4
2	C	474	ASP	2.3
2	C	188	LYS	2.3
1	B	288	SER	2.3
1	B	259	TYR	2.3
1	B	126	LYS	2.3
2	C	322	ASN	2.3
1	B	253	THR	2.3
1	B	314	GLN	2.3
1	B	7	ILE	2.2
1	B	287	MET	2.2
2	C	469	ALA	2.2
2	C	327	GLU	2.2
1	B	245	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	294	PRO	2.1
1	B	179	ILE	2.1
1	B	230	THR	2.1
1	B	228	PRO	2.1
1	B	423	THR	2.1
2	C	154	ASN	2.1
1	B	401	ILE	2.0
1	B	54	ARG	2.0
1	B	356	ILE	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(Å ²)	Q<0.9
3	PRO	B	504	7/8	0.85	0.23	97,101,108,109	0
3	PRO	C	603	7/8	0.86	0.28	64,69,80,80	0
3	PRO	B	505	7/8	0.87	0.19	68,75,86,86	0
3	PRO	B	502	7/8	0.88	0.20	58,60,68,75	0
3	PRO	B	503	7/8	0.91	0.15	46,54,73,83	0
3	PRO	B	501	7/8	0.95	0.14	68,77,82,83	0
3	PRO	C	604	7/8	0.95	0.19	59,69,78,82	7
4	MN	C	601	1/1	0.98	0.16	66,66,66,66	0
4	MN	C	602	1/1	0.99	0.10	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.