Full wwPDB X-ray Structure Validation Report ⓘ

Jun 6, 2024 – 10:13 AM EDT

PDB ID	:	8U7B
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:

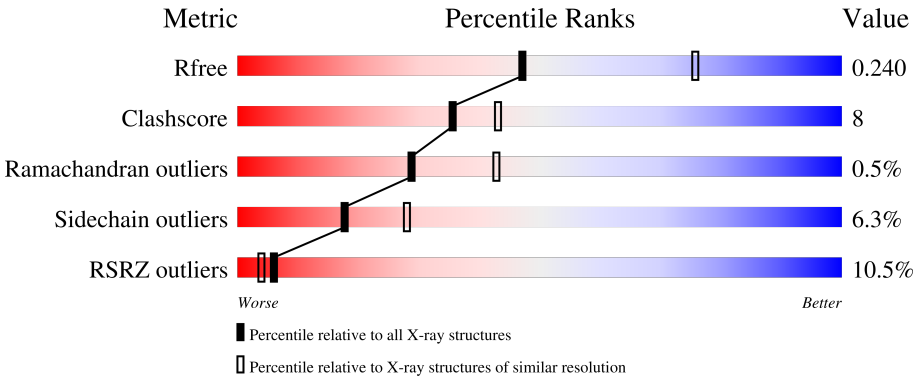
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 <=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	13% 70% 22% · 6%
2	C	507	8% 82% 17% ·

2 Entry composition

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.

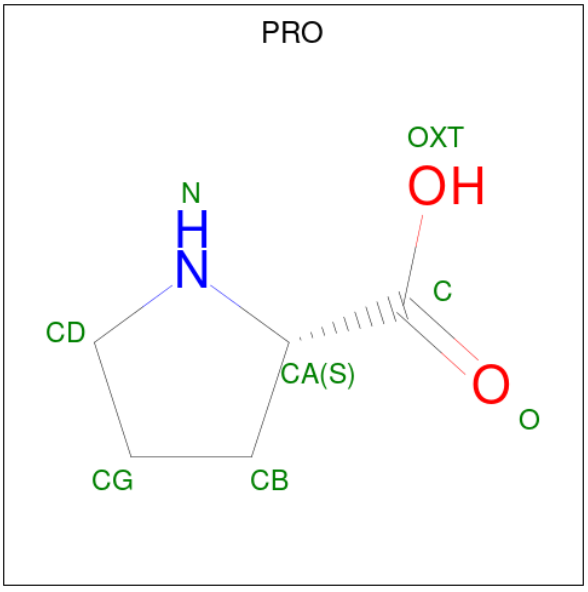
- Molecule 1 is a protein called TIR domain-containing protein.

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

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

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

- Molecule 3 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$).



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

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 5 is water.

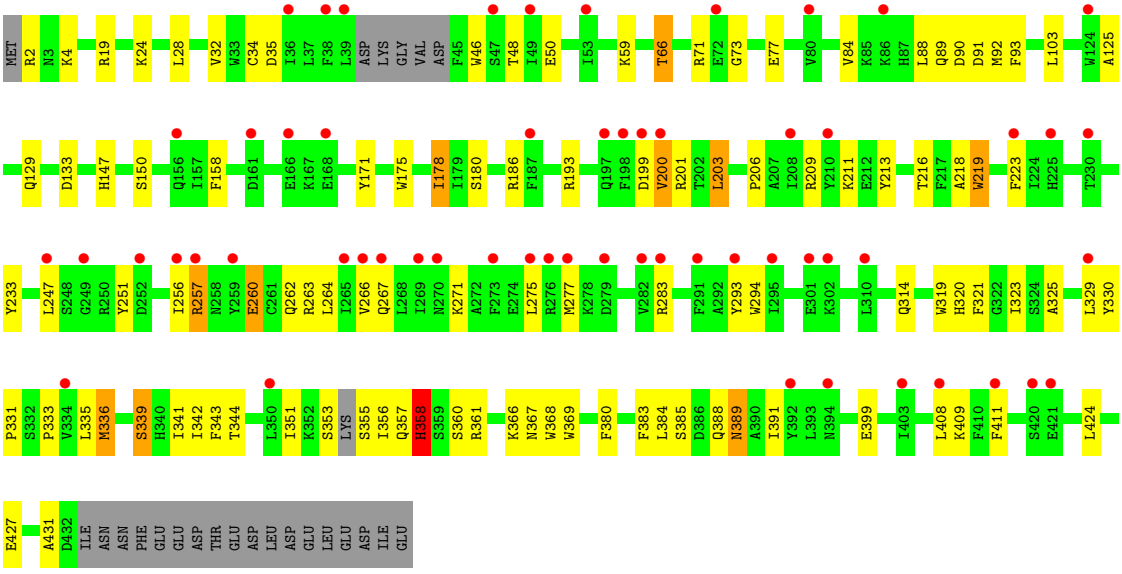
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	37	Total O 37 37	0	0
5	C	54	Total O 54 54	0	0

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.

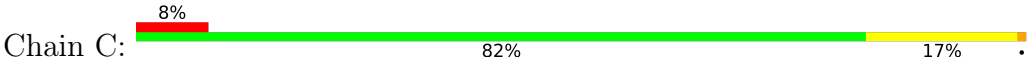
• Molecule 1: TIR domain-containing protein

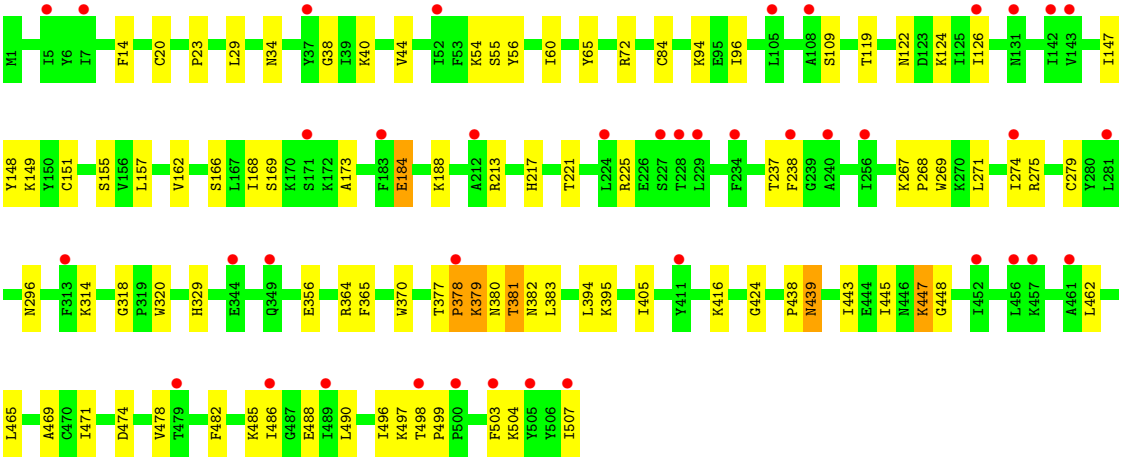
Chain B:



• Molecule 2: Piwi domain-containing protein

Chain C:





4 Data and refinement statistics (i)

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 – 2.66 170.76 – 2.66	Depositor EDS
% Data completeness (in resolution range)	67.6 (49.71-2.66) 67.6 (170.76-2.66)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.20rc3_4406: ???)	Depositor
R, R_{free}	0.179 , 0.239 0.186 , 0.240	Depositor DCC
R_{free} test set	2070 reflections (5.06%)	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)	0.35 , 67.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.49	0/4695
2	C	0.30	0/4099	0.48	0/5571
All	All	0.30	0/7554	0.48	0/10266

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	B	3369	0	3157	65	0
2	C	3996	0	3904	56	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
5	C	54	0	0	2	0
All	All	7507	0	7110	117	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 8.

All (117) 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	0.93
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
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
2:C:370:TRP:CD1	2:C:447:LYS:HG2	2.43	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:199:ASP:C	1:B:201:ARG:H	2.14	0.51
1:B:263:ARG:O	1:B:267:GLN:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:355:SER:O	1:B:356:ILE:C	2.51	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: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: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
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:247:LEU:HD22	1:B:329:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:314:LYS:NZ	2:C:496:ILE:O	2.47	0.44
1:B:200:VAL:O	1:B:203:LEU:HD21	2.18	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: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
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:211:LYS:C	1:B:213:TYR:H	2.25	0.40
1:B:330:TYR:CD1	1:B:331:PRO:HA	2.57	0.40
2:C:498:THR:HA	2:C:499:PRO:HD3	1.95	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%)	22	33
2	C	505/507 (100%)	472 (94%)	31 (6%)	2 (0%)	34	48
All	All	923/956 (96%)	862 (93%)	56 (6%)	5 (0%)	29	43

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 (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	B	345/414 (83%)	317 (92%)	28 (8%)	11	17
2	C	413/446 (93%)	393 (95%)	20 (5%)	25	39
All	All	758/860 (88%)	710 (94%)	48 (6%)	18	28

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2	ARG

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Mol	Chain	Res	Type
1	B	32	VAL
1	B	34	CYS
1	B	48	THR
1	B	66	THR
1	B	71	ARG
1	B	89	GLN
1	B	91	ASP
1	B	92	MET
1	B	133	ASP
1	B	150	SER
1	B	178	ILE
1	B	180	SER
1	B	186	ARG
1	B	203	LEU
1	B	219	TRP
1	B	257	ARG
1	B	260	GLU
1	B	314	GLN
1	B	336	MET
1	B	339	SER
1	B	358	HIS
1	B	383	PHE
1	B	384	LEU
1	B	389	ASN
1	B	408	LEU
1	B	409	LYS
1	B	411	PHE
2	C	40	LYS
2	C	44	VAL
2	C	109	SER
2	C	149	LYS
2	C	155	SER
2	C	166	SER
2	C	169	SER
2	C	184	GLU
2	C	221	THR
2	C	279	CYS
2	C	296	ASN
2	C	380	ASN
2	C	381	THR
2	C	439	ASN
2	C	443	ILE

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Mol	Chain	Res	Type
2	C	447	LYS
2	C	474	ASP
2	C	488	GLU
2	C	497	LYS
2	C	503	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	340	HIS
1	B	389	ASN
2	C	329	HIS

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 monosaccharides 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	501	-	5,7,8	0.53	0	7,8,10	1.31	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PRO	B	504	-	5,7,8	0.50	0	7,8,10	1.26	1 (14%)
3	PRO	B	505	-	5,7,8	0.49	0	7,8,10	1.25	1 (14%)
3	PRO	B	503	-	5,7,8	0.52	0	7,8,10	1.28	1 (14%)
3	PRO	C	604	-	5,7,8	0.57	0	7,8,10	1.13	0
3	PRO	B	502	-	5,7,8	0.51	0	7,8,10	1.34	1 (14%)
3	PRO	C	603	-	5,7,8	0.54	0	7,8,10	1.19	0

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	501	-	-	0/0/9/11	0/1/1/1
3	PRO	B	504	-	-	0/0/9/11	0/1/1/1
3	PRO	B	505	-	-	0/0/9/11	0/1/1/1
3	PRO	B	503	-	-	0/0/9/11	0/1/1/1
3	PRO	C	604	-	-	0/0/9/11	0/1/1/1
3	PRO	B	502	-	-	0/0/9/11	0/1/1/1
3	PRO	C	603	-	-	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(^{o})	Ideal(^{o})
3	B	502	PRO	O-C-CA	-2.27	118.83	124.78
3	B	503	PRO	O-C-CA	-2.22	118.95	124.78
3	B	504	PRO	O-C-CA	-2.06	119.38	124.78
3	B	505	PRO	O-C-CA	-2.06	119.38	124.78
3	B	501	PRO	O-C-CA	-2.01	119.50	124.78

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	504	PRO	1	0
3	B	505	PRO	1	0
3	C	603	PRO	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	0.88	58 (13%) 3 2	32, 78, 111, 162	1 (0%)
2	C	507/507 (100%)	0.92	40 (7%) 12 10	28, 59, 100, 144	5 (0%)
All	All	931/956 (97%)	0.90	98 (10%) 6 4	28, 68, 108, 162	6 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	LEU	5.4
1	B	266	VAL	4.8
1	B	197	GLN	4.5
1	B	279	ASP	4.2
1	B	198	PHE	4.1
1	B	168	GLU	4.0
1	B	420	SER	3.8
1	B	282	VAL	3.8
1	B	302	LYS	3.6
1	B	295	ILE	3.5
2	C	507	ILE	3.5
2	C	131	ASN	3.4
2	C	52	ILE	3.4
1	B	36	ILE	3.3
2	C	37	TYR	3.3
2	C	452	ILE	3.2
1	B	166	GLU	3.2
2	C	344	GLU	3.2
2	C	500	PRO	3.1
1	B	210	TYR	3.1
1	B	277	MET	3.0
2	C	411	TYR	3.0
1	B	38	PHE	3.0
1	B	293	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	408	LEU	2.9
2	C	238	PHE	2.9
2	C	234	PHE	2.9
2	C	171	SER	2.9
2	C	227	SER	2.9
2	C	183	PHE	2.8
1	B	301	GLU	2.8
1	B	200	VAL	2.8
2	C	313	PHE	2.8
1	B	225	HIS	2.7
1	B	247	LEU	2.7
1	B	270	ASN	2.7
1	B	275	LEU	2.7
2	C	486	ILE	2.7
1	B	291	PHE	2.7
1	B	334	VAL	2.7
2	C	5	ILE	2.7
1	B	269	ILE	2.6
1	B	156	GLN	2.6
1	B	267	GLN	2.6
1	B	49	ILE	2.6
1	B	86	LYS	2.5
2	C	212	ALA	2.5
2	C	142	ILE	2.5
1	B	249	GLY	2.5
1	B	259	TYR	2.5
1	B	161	ASP	2.5
2	C	461	ALA	2.5
1	B	47	SER	2.5
2	C	503	PHE	2.5
2	C	457	LYS	2.5
2	C	108	ALA	2.4
1	B	329	LEU	2.4
2	C	7	ILE	2.4
1	B	411	PHE	2.4
1	B	350	LEU	2.4
2	C	256	ILE	2.3
2	C	498	THR	2.3
1	B	72	GLU	2.3
2	C	105	LEU	2.3
2	C	456	LEU	2.3
1	B	252	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	229	LEU	2.2
2	C	378	PRO	2.2
1	B	273	PHE	2.2
1	B	53	ILE	2.2
1	B	80	VAL	2.2
2	C	126	ILE	2.2
1	B	392	TYR	2.2
2	C	505	TYR	2.2
1	B	256	ILE	2.2
2	C	274	ILE	2.2
1	B	124	TRP	2.2
2	C	489	ILE	2.1
2	C	349	GLN	2.1
1	B	403	ILE	2.1
2	C	143	VAL	2.1
1	B	283	ARG	2.1
1	B	394	ASN	2.1
1	B	230	THR	2.1
2	C	240	ALA	2.1
1	B	276	ARG	2.1
2	C	224	LEU	2.1
1	B	208	ILE	2.1
1	B	187	PHE	2.1
1	B	257	ARG	2.0
1	B	199	ASP	2.0
1	B	421	GLU	2.0
1	B	223	PHE	2.0
1	B	265	ILE	2.0
2	C	228	THR	2.0
2	C	479	THR	2.0
1	B	310	LEU	2.0
2	C	281	LEU	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 monosaccharides 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, 95^{th} 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	0.90	0.15	97,101,108,109	0
3	PRO	C	604	7/8	0.93	0.22	59,69,78,82	7
3	PRO	B	501	7/8	0.94	0.38	68,77,82,83	0
3	PRO	B	505	7/8	0.94	0.18	68,75,86,86	0
3	PRO	C	603	7/8	0.94	0.22	64,69,80,80	0
3	PRO	B	503	7/8	0.94	0.21	46,54,73,83	0
3	PRO	B	502	7/8	0.98	0.20	58,60,68,75	0
4	MN	C	601	1/1	0.98	0.31	66,66,66,66	0
4	MN	C	602	1/1	0.99	0.25	67,67,67,67	0

6.5 Other polymers (i)

There are no such residues in this entry.