



Full wwPDB X-ray Structure Validation Report

May 21, 2020 – 07:49 am BST

PDB ID : 4RL5
Title : Crystal structure of the Arabidopsis exocyst subunit exo70 family protein A1
Authors : Zhang, Z.-M.; Zhang, C.; Song, J.
Deposited on : 2014-10-15
Resolution : 3.10 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 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 : 2.11
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) : 2.11

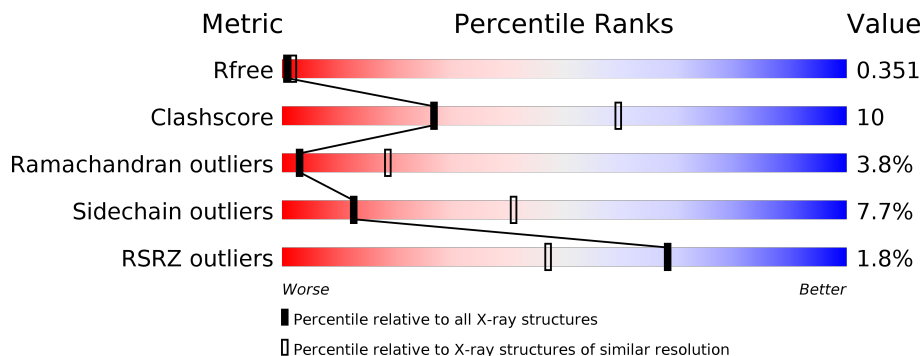
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 on 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	565	
1	B	565	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6415 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 Exocyst complex component EXO70A1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	448	3197	2034	550	598	3	12	0	0	0
1	B	468	3218	2027	557	619	3	12	0	0	0

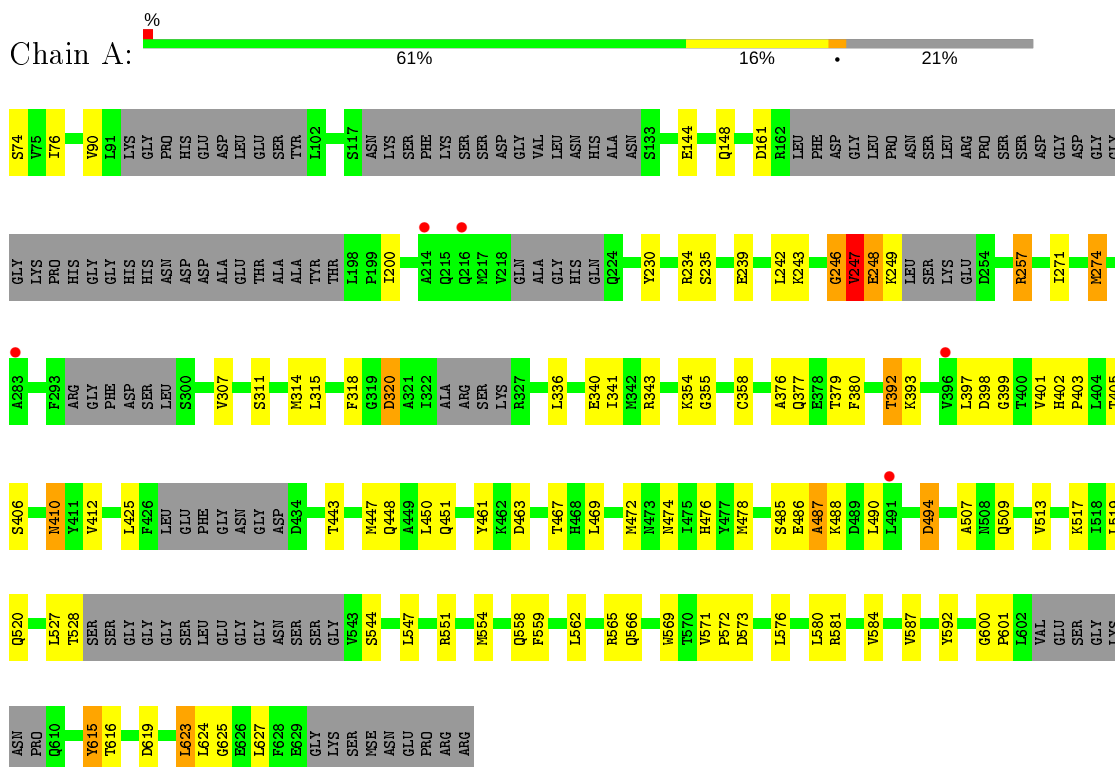
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	SER	-	EXPRESSION TAG	UNP Q9LZD3
B	74	SER	-	EXPRESSION TAG	UNP Q9LZD3

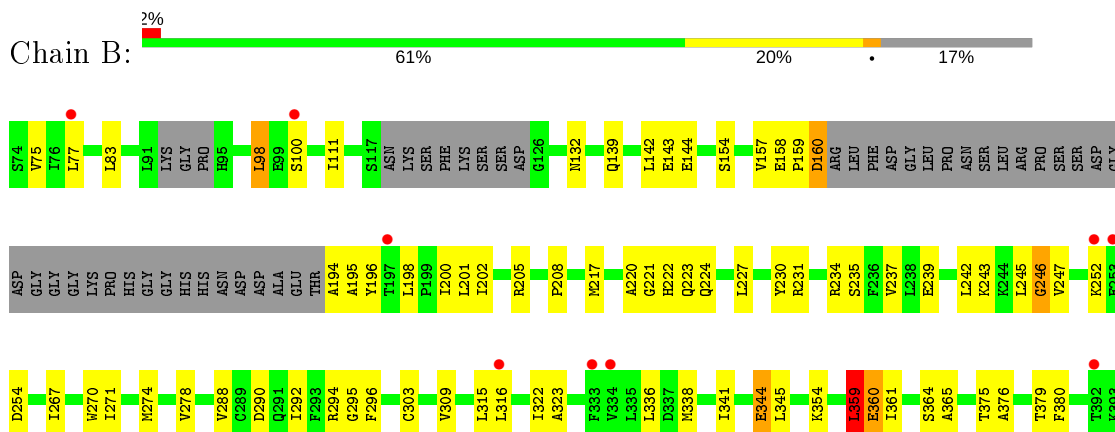
3 Residue-property plots

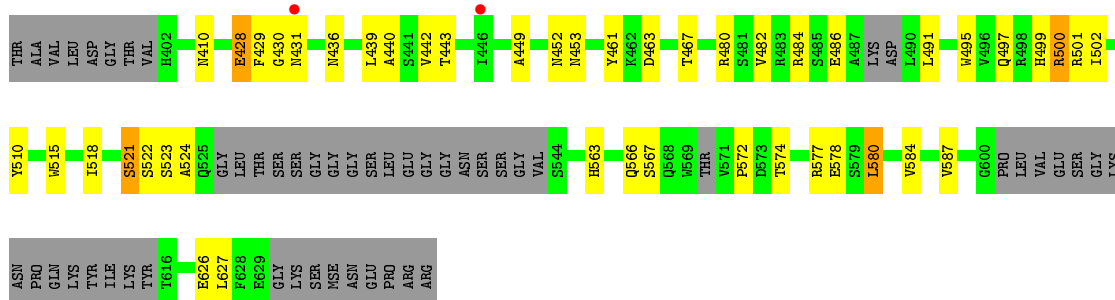
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Exocyst complex component EXO70A1



- Molecule 1: Exocyst complex component EXO70A1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.11Å 72.12Å 327.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.52 – 3.10 48.52 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.52-3.10) 82.8 (48.52-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 3.01Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.324 , 0.348 0.328 , 0.351	Depositor DCC
R_{free} test set	1986 reflections (7.36%)	wwPDB-VP
Wilson B-factor (Å ²)	70.1	Xtrriage
Anisotropy	0.996	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 79.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	6415	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% 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	0.23	0/3229	0.44	0/4373
1	B	0.23	0/3252	0.45	0/4420
All	All	0.23	0/6481	0.44	0/8793

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 [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	3197	0	2824	66	0
1	B	3218	0	2702	56	0
All	All	6415	0	5526	122	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 10.

All (122) 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:247:VAL:CG2	1:A:314:MSE:SE	2.78	0.82
1:B:274:MSE:HE1	1:B:315:LEU:HB3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:HIS:HD1	1:A:403:PRO:HD2	1.53	0.73
1:B:428:GLU:O	1:B:430:GLY:N	2.21	0.72
1:A:246:GLY:O	1:A:247:VAL:HG12	1.90	0.71
1:A:247:VAL:HG23	1:A:314:MSE:CE	2.23	0.68
1:A:401:VAL:HG23	1:A:572:PRO:HG2	1.77	0.67
1:A:528:THR:HG23	1:A:547:LEU:HD12	1.75	0.67
1:A:565:ARG:HG3	1:A:566:GLN:HG3	1.76	0.67
1:B:154:SER:OG	1:B:234:ARG:NH1	2.27	0.66
1:A:247:VAL:HG22	1:A:314:MSE:SE	2.47	0.64
1:A:247:VAL:O	1:A:249:LYS:N	2.28	0.63
1:A:469:LEU:HA	1:A:472:MSE:HE3	1.81	0.62
1:A:247:VAL:CG2	1:A:314:MSE:CE	2.77	0.61
1:A:248:GLU:CB	1:A:318:PHE:HB2	2.31	0.61
1:A:376:ALA:O	1:A:379:THR:OG1	2.17	0.60
1:A:486:GLU:HA	1:A:487:ALA:HB3	1.81	0.60
1:B:252:LYS:H	1:B:254:ASP:H	1.48	0.60
1:A:448:GLN:OE1	1:A:451:GLN:NE2	2.34	0.60
1:B:515:TRP:HE3	1:B:518:ILE:HG21	1.66	0.60
1:B:271:ILE:HG23	1:B:341:ILE:HG13	1.84	0.59
1:A:472:MSE:HE2	1:A:507:ALA:HA	1.83	0.59
1:A:405:THR:HG23	1:A:450:LEU:HD21	1.85	0.59
1:A:242:LEU:HD22	1:A:311:SER:HB3	1.83	0.58
1:A:247:VAL:HG21	1:A:314:MSE:SE	2.54	0.57
1:A:616:THR:H	1:A:619:ASP:HB2	1.70	0.57
1:A:447:MSE:HB3	1:A:478:MSE:HE3	1.88	0.56
1:B:267:ILE:HG23	1:B:338:MSE:HE3	1.88	0.56
1:A:243:LYS:HA	1:A:247:VAL:HB	1.89	0.55
1:B:202:ILE:HG21	1:B:234:ARG:NH2	2.22	0.54
1:B:567:SER:HA	1:B:627:LEU:HA	1.88	0.54
1:A:461:TYR:HB2	1:A:467:THR:HG22	1.89	0.54
1:B:359:LEU:O	1:B:361:ILE:N	2.37	0.52
1:A:235:SER:HB2	1:A:307:VAL:HA	1.91	0.52
1:B:242:LEU:HD23	1:B:245:LEU:HD21	1.90	0.52
1:B:336:LEU:HD11	1:B:376:ALA:HB2	1.91	0.52
1:A:402:HIS:HB2	1:A:474:ASN:HD21	1.75	0.52
1:B:376:ALA:O	1:B:379:THR:OG1	2.18	0.52
1:A:412:VAL:HG21	1:A:443:THR:HG23	1.91	0.51
1:A:247:VAL:HG23	1:A:314:MSE:HE3	1.93	0.51
1:B:361:ILE:O	1:B:364:SER:OG	2.22	0.51
1:B:482:VAL:HG11	1:B:495:TRP:CZ3	2.46	0.50
1:B:574:THR:HG22	1:B:577:ARG:HH21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:GLU:HG3	1:B:345:LEU:HG	1.94	0.49
1:B:278:VAL:HG21	1:B:345:LEU:HD13	1.95	0.49
1:A:271:ILE:HG23	1:A:341:ILE:HG12	1.94	0.49
1:B:449:ALA:HA	1:B:452:ASN:ND2	2.27	0.49
1:A:74:SER:O	1:A:76:ILE:N	2.41	0.49
1:A:486:GLU:HA	1:A:488:LYS:H	1.78	0.48
1:A:274:MSE:HE2	1:A:315:LEU:HB3	1.96	0.48
1:B:222:HIS:O	1:B:224:GLN:N	2.44	0.48
1:A:402:HIS:ND1	1:A:403:PRO:HD2	2.23	0.48
1:B:83:LEU:HG	1:B:111:ILE:HG21	1.96	0.48
1:B:159:PRO:HA	1:B:160:ASP:HA	1.55	0.47
1:A:527:LEU:HD21	1:A:551:ARG:HE	1.80	0.47
1:A:247:VAL:O	1:A:247:VAL:HG13	2.14	0.47
1:B:359:LEU:C	1:B:361:ILE:H	2.17	0.47
1:A:469:LEU:HD22	1:A:569:TRP:CE3	2.50	0.47
1:A:463:ASP:OD1	1:A:463:ASP:N	2.46	0.47
1:B:246:GLY:HA3	1:B:247:VAL:HA	1.60	0.47
1:B:452:ASN:OD1	1:B:453:ASN:N	2.47	0.47
1:B:227:LEU:HD22	1:B:303:CYS:HB2	1.96	0.46
1:B:440:ALA:HA	1:B:443:THR:HG22	1.97	0.46
1:B:323:ALA:O	1:B:375:THR:HG21	2.16	0.46
1:A:509:GLN:O	1:A:513:VAL:HG22	2.15	0.46
1:A:584:VAL:HA	1:A:587:VAL:HG22	1.96	0.46
1:A:573:ASP:HB3	1:A:576:LEU:HB3	1.98	0.46
1:B:375:THR:O	1:B:379:THR:HG23	2.16	0.45
1:B:449:ALA:HA	1:B:452:ASN:HD21	1.82	0.45
1:B:270:TRP:CZ2	1:B:274:MSE:HE3	2.51	0.45
1:B:497:GLN:HG2	1:B:500:ARG:HH11	1.80	0.45
1:A:230:TYR:O	1:A:234:ARG:HB2	2.16	0.45
1:A:581:ARG:HD3	1:A:625:GLY:HA2	1.98	0.45
1:B:194:ALA:HA	1:B:195:ALA:C	2.37	0.45
1:B:270:TRP:CE3	1:B:338:MSE:HE2	2.52	0.44
1:A:406:SER:O	1:A:410:ASN:HB2	2.16	0.44
1:B:499:HIS:O	1:B:502:ILE:HG22	2.18	0.44
1:B:463:ASP:OD1	1:B:463:ASP:N	2.47	0.44
1:A:354:LYS:HB3	1:A:355:GLY:H	1.52	0.44
1:A:398:ASP:OD1	1:A:399:GLY:N	2.50	0.43
1:B:98:LEU:O	1:B:100:SER:N	2.49	0.43
1:A:592:TYR:OH	1:A:615:TYR:O	2.33	0.43
1:A:485:SER:OG	1:A:486:GLU:N	2.50	0.43
1:A:392:THR:HA	1:A:393:LYS:HA	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:GLU:HA	1:B:159:PRO:HD3	1.93	0.43
1:B:230:TYR:CE1	1:B:234:ARG:HG3	2.54	0.43
1:B:231:ARG:O	1:B:235:SER:HB3	2.18	0.43
1:A:476:HIS:NE2	1:A:573:ASP:OD2	2.33	0.43
1:A:527:LEU:HA	1:A:528:THR:HA	1.52	0.42
1:B:359:LEU:O	1:B:361:ILE:HG12	2.19	0.42
1:A:320:ASP:OD1	1:A:320:ASP:N	2.52	0.42
1:A:397:LEU:HB3	1:A:398:ASP:H	1.56	0.42
1:B:436:ASN:O	1:B:439:LEU:HB3	2.19	0.42
1:B:515:TRP:CE2	1:B:584:VAL:HG21	2.54	0.42
1:B:220:ALA:HB3	1:B:221:GLY:HA2	2.02	0.42
1:B:461:TYR:HE2	1:B:467:THR:HA	1.83	0.42
1:A:494:ASP:OD1	1:A:494:ASP:N	2.52	0.42
1:A:600:GLY:HA2	1:A:601:PRO:HA	1.91	0.42
1:A:554:MSE:HE3	1:A:558:GLN:NE2	2.35	0.42
1:B:230:TYR:CE1	1:B:288:VAL:HG22	2.55	0.42
1:B:584:VAL:HA	1:B:587:VAL:HG22	2.01	0.42
1:B:521:SER:O	1:B:523:SER:N	2.53	0.42
1:A:377:GLN:O	1:A:380:PHE:HB2	2.20	0.41
1:A:401:VAL:HA	1:A:474:ASN:OD1	2.18	0.41
1:A:517:LYS:O	1:A:520:GLN:HG2	2.21	0.41
1:B:143:GLU:HG2	1:B:217:MSE:HE3	2.00	0.41
1:B:239:GLU:O	1:B:243:LYS:HG3	2.20	0.41
1:B:580:LEU:O	1:B:584:VAL:HG12	2.21	0.41
1:A:448:GLN:HA	1:A:451:GLN:HE21	1.84	0.41
1:B:510:TYR:OH	1:B:566:GLN:OE1	2.38	0.41
1:A:247:VAL:C	1:A:249:LYS:N	2.73	0.41
1:A:341:ILE:HD12	1:A:341:ILE:HA	1.88	0.41
1:B:316:LEU:HD21	1:B:365:ALA:HB2	2.02	0.41
1:A:239:GLU:O	1:A:243:LYS:HG3	2.21	0.41
1:A:624:LEU:HA	1:A:624:LEU:HD23	1.92	0.41
1:A:486:GLU:HA	1:A:488:LYS:N	2.36	0.41
1:B:294:ARG:O	1:B:296:PHE:N	2.54	0.41
1:A:336:LEU:O	1:A:340:GLU:HG3	2.21	0.40
1:B:439:LEU:O	1:B:442:VAL:HG12	2.22	0.40
1:A:271:ILE:HD12	1:A:341:ILE:HG21	2.04	0.40
1:A:559:PHE:CE2	1:A:623:LEU:HD13	2.56	0.40
1:B:205:ARG:O	1:B:208:PRO:HD2	2.21	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	426/565 (75%)	381 (89%)	32 (8%)	13 (3%)	4	23
1	B	452/565 (80%)	406 (90%)	26 (6%)	20 (4%)	2	15
All	All	878/1130 (78%)	787 (90%)	58 (7%)	33 (4%)	3	19

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	ASP
1	A	200	ILE
1	A	248	GLU
1	B	157	VAL
1	B	292	ILE
1	B	359	LEU
1	B	486	GLU
1	B	572	PRO
1	A	392	THR
1	B	200	ILE
1	B	246	GLY
1	B	295	GLY
1	B	354	LYS
1	B	360	GLU
1	B	429	PHE
1	B	521	SER
1	B	522	SER
1	A	358	CYS
1	A	544	SER
1	A	615	TYR
1	B	98	LEU
1	B	196	TYR
1	B	431	ASN
1	A	247	VAL
1	A	487	ALA

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Mol	Chain	Res	Type
1	B	75	VAL
1	B	524	ALA
1	A	246	GLY
1	A	490	LEU
1	B	223	GLN
1	B	428	GLU
1	A	257	ARG
1	A	90	VAL

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	280/479 (58%)	264 (94%)	16 (6%)	20	52
1	B	264/479 (55%)	238 (90%)	26 (10%)	8	29
All	All	544/958 (57%)	502 (92%)	42 (8%)	13	41

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	GLU
1	A	148	GLN
1	A	247	VAL
1	A	257	ARG
1	A	274	MSE
1	A	320	ASP
1	A	343	ARG
1	A	410	ASN
1	A	425	LEU
1	A	494	ASP
1	A	519	LEU
1	A	562	LEU
1	A	571	VAL
1	A	580	LEU
1	A	623	LEU

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Mol	Chain	Res	Type
1	A	627	LEU
1	B	77	LEU
1	B	132	ASN
1	B	139	GLN
1	B	142	LEU
1	B	144	GLU
1	B	160	ASP
1	B	198	LEU
1	B	201	LEU
1	B	237	VAL
1	B	290	ASP
1	B	309	VAL
1	B	322	ILE
1	B	344	GLU
1	B	359	LEU
1	B	360	GLU
1	B	380	PHE
1	B	410	ASN
1	B	480	ARG
1	B	484	ARG
1	B	491	LEU
1	B	500	ARG
1	B	501	ARG
1	B	563	HIS
1	B	578	GLU
1	B	580	LEU
1	B	626	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	451	GLN
1	A	474	ASN

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 carbohydrates 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	435/565 (76%)	-0.17	5 (1%) 80 64	50, 99, 143, 171	0
1	B	455/565 (80%)	-0.16	11 (2%) 59 37	82, 117, 147, 164	0
All	All	890/1130 (78%)	-0.16	16 (1%) 68 47	50, 111, 146, 171	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	252	LYS	4.6
1	A	216	GLN	3.7
1	A	283	ALA	3.2
1	B	100	SER	3.1
1	B	333	PHE	3.1
1	B	334	VAL	2.5
1	B	77	LEU	2.5
1	B	431	ASN	2.5
1	B	253	GLU	2.4
1	B	197	THR	2.3
1	A	214	ALA	2.3
1	A	396	VAL	2.2
1	B	392	THR	2.1
1	A	491	LEU	2.1
1	B	316	LEU	2.0
1	B	446	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 carbohydrates 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.