



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:54 PM UTC

PDB ID : 4GKW / pdb_00004gkw
Title : Crystal Structure of the Coiled-coil Domain of C. elegans SAS-6
Authors : Qiao, R.; Dong, G.
Deposited on : 2012-08-13
Resolution : 3.30 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

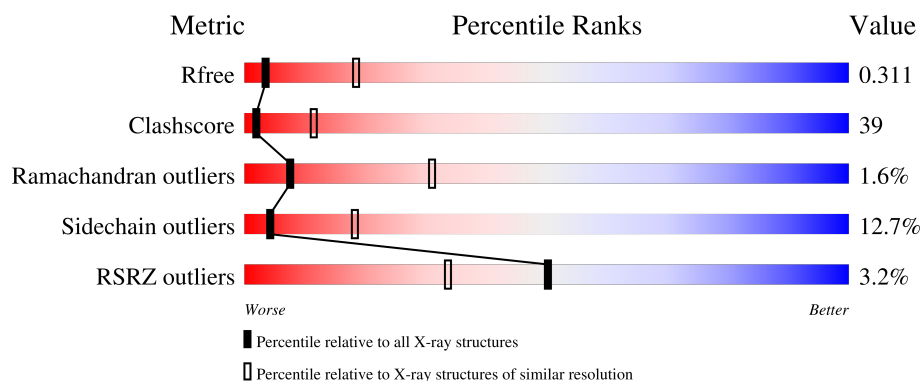
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	167	2% 38% 49% 7% 5%
1	B	167	4% 29% 51% 13% 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2578 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 Spindle assembly abnormal protein 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	0	0	0
			1289	781	233	270	5			
1	B	158	Total	C	N	O	S	0	0	0
			1289	781	233	270	5			

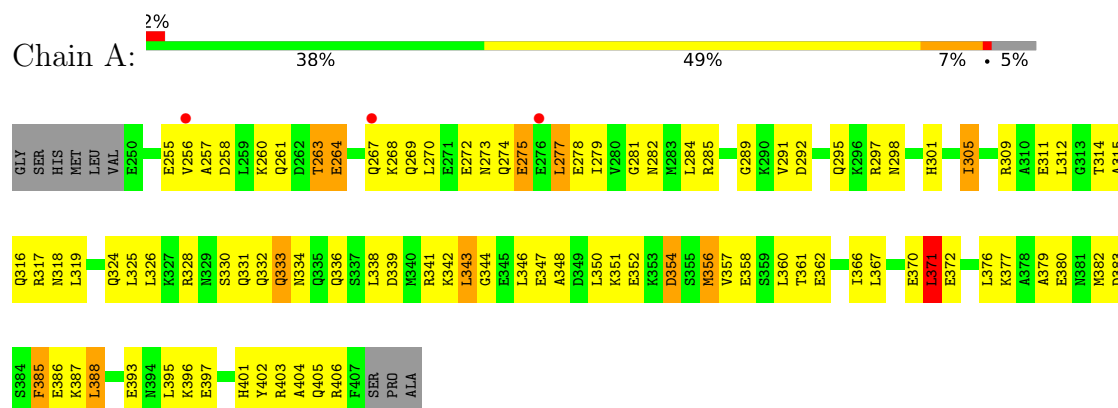
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	GLY	-	expression tag	UNP O62479
A	245	SER	-	expression tag	UNP O62479
A	246	HIS	-	expression tag	UNP O62479
A	247	MET	-	expression tag	UNP O62479
B	244	GLY	-	expression tag	UNP O62479
B	245	SER	-	expression tag	UNP O62479
B	246	HIS	-	expression tag	UNP O62479
B	247	MET	-	expression tag	UNP O62479

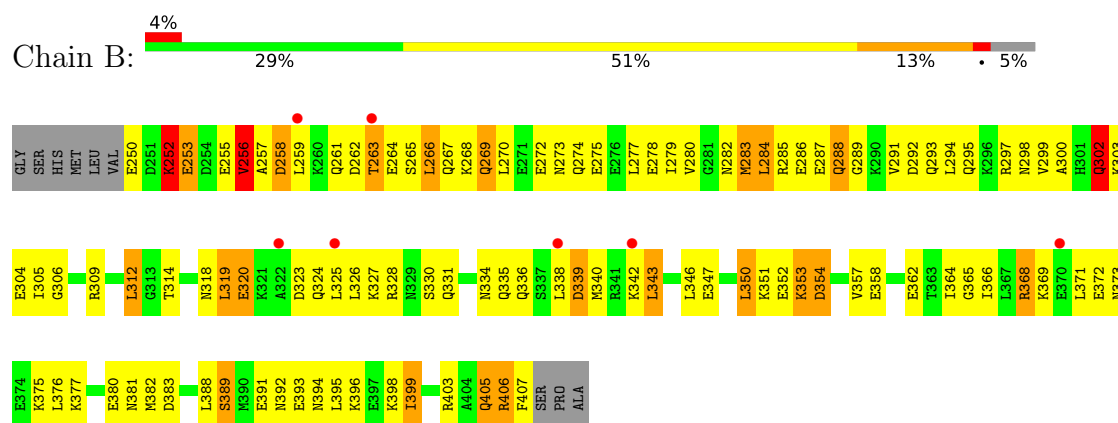
3 Residue-property plots

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: Spindle assembly abnormal protein 6



• Molecule 1: Spindle assembly abnormal protein 6



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	140.29 Å 140.29 Å 74.67 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 3.30 25.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	92.9 (25.00-3.30) 92.7 (25.00-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.91 (at 2.99 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.258 , 0.299 0.269 , 0.311	Depositor DCC
R_{free} test set	2376 reflections (7.24%)	wwPDB-VP
Wilson B-factor (Å ²)	67.9	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 99.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.033 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2578	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.12% 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	0.58	0/1293	1.03	7/1719 (0.4%)
1	B	0.56	0/1293	1.12	11/1719 (0.6%)
All	All	0.57	0/2586	1.08	18/3438 (0.5%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	406	ARG	N-CA-C	8.61	122.90	111.28
1	B	293	GLN	N-CA-C	8.36	120.17	111.14
1	B	288	GLN	N-CA-C	-7.31	104.34	113.18
1	A	324	GLN	N-CA-C	-6.77	103.90	111.28
1	A	371	LEU	N-CA-C	-6.71	104.04	111.82
1	B	300	ALA	N-CA-C	-6.51	104.22	111.71
1	B	351	LYS	N-CA-C	-6.48	104.30	111.82
1	B	319	LEU	N-CA-C	-6.29	105.58	113.18
1	A	343	LEU	N-CA-C	-6.21	104.41	112.23
1	B	339	ASP	N-CA-C	5.85	118.89	111.69
1	B	375	LYS	N-CA-C	-5.85	105.24	112.90
1	A	289	GLY	N-CA-C	-5.55	105.78	112.49
1	A	333	GLN	N-CA-C	-5.51	106.05	112.89
1	A	305	ILE	N-CA-C	-5.47	105.01	113.16
1	A	264	GLU	N-CA-C	-5.43	105.00	111.03
1	B	269	GLN	N-CA-C	-5.21	105.60	111.28
1	B	263	THR	N-CA-C	-5.07	106.36	112.54
1	B	302	GLN	N-CA-C	-5.02	105.81	111.28

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	A	1289	0	1288	110	0
1	B	1289	0	1288	137	0
All	All	2578	0	2576	199	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 39.

All (199) 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:263:THR:HG23	1:B:263:THR:HG22	1.34	1.09
1:A:270:LEU:HD11	1:B:269:GLN:HB2	1.40	1.02
1:B:392:ASN:HD21	1:B:396:LYS:HE3	1.30	0.94
1:A:346:LEU:HD13	1:B:346:LEU:HD22	1.54	0.90
1:A:263:THR:CG2	1:B:263:THR:HG22	2.02	0.89
1:B:284:LEU:O	1:B:288:GLN:HG2	1.73	0.88
1:A:351:LYS:HA	1:A:354:ASP:HB2	1.58	0.85
1:B:314:THR:O	1:B:318:ASN:HB2	1.75	0.85
1:B:406:ARG:HG2	1:B:406:ARG:HH11	1.42	0.84
1:A:338:LEU:HD22	1:A:342:LYS:HE3	1.63	0.80
1:A:305:ILE:HG12	1:B:305:ILE:HG12	1.61	0.80
1:B:289:GLY:HA2	1:B:292:ASP:OD2	1.82	0.79
1:B:392:ASN:ND2	1:B:396:LYS:HE3	1.99	0.78
1:B:264:GLU:O	1:B:268:LYS:HE2	1.84	0.78
1:A:350:LEU:HD23	1:B:350:LEU:HG	1.66	0.77
1:A:346:LEU:HB3	1:B:346:LEU:CD2	2.14	0.77
1:B:272:GLU:HA	1:B:275:GLU:OE1	1.85	0.77
1:B:291:VAL:O	1:B:295:GLN:HB2	1.84	0.77
1:A:274:GLN:HG2	1:B:273:ASN:HD21	1.49	0.77
1:A:298:ASN:HD21	1:B:297:ARG:HB3	1.51	0.75
1:A:350:LEU:HA	1:B:350:LEU:HD21	1.67	0.75
1:A:277:LEU:HA	1:B:277:LEU:HD23	1.70	0.74
1:A:274:GLN:HG2	1:B:273:ASN:ND2	2.03	0.73
1:A:311:GLU:HB3	1:B:312:LEU:HD11	1.70	0.73
1:A:346:LEU:HB3	1:B:346:LEU:HD21	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:LEU:O	1:B:323:ASP:HB2	1.89	0.71
1:A:405:GLN:O	1:A:406:ARG:HD3	1.91	0.71
1:A:263:THR:HG23	1:B:263:THR:CG2	2.18	0.70
1:A:318:ASN:HB3	1:B:319:LEU:HD11	1.73	0.69
1:A:305:ILE:HG12	1:B:305:ILE:CG1	2.21	0.69
1:A:388:LEU:HD13	1:B:388:LEU:HG	1.75	0.68
1:A:273:ASN:OD1	1:B:273:ASN:HB3	1.93	0.68
1:A:331:GLN:HA	1:A:334:ASN:ND2	2.09	0.68
1:B:319:LEU:O	1:B:319:LEU:HD23	1.94	0.67
1:A:298:ASN:HD22	1:B:297:ARG:HD2	1.59	0.66
1:A:319:LEU:HD13	1:A:319:LEU:O	1.95	0.66
1:A:295:GLN:HG2	1:B:294:LEU:CD1	2.26	0.66
1:B:325:LEU:HG	1:B:328:ARG:HH12	1.59	0.65
1:B:399:ILE:O	1:B:403:ARG:HG3	1.96	0.65
1:B:406:ARG:O	1:B:406:ARG:HG3	1.97	0.65
1:A:301:HIS:O	1:A:305:ILE:HG13	1.98	0.64
1:A:312:LEU:O	1:A:316:GLN:HG3	1.97	0.64
1:A:298:ASN:ND2	1:B:297:ARG:HD2	2.13	0.64
1:B:277:LEU:HD13	1:B:277:LEU:O	1.99	0.63
1:B:346:LEU:O	1:B:346:LEU:HD23	1.99	0.62
1:A:295:GLN:HE21	1:B:294:LEU:HD11	1.64	0.62
1:A:256:VAL:HG13	1:B:259:LEU:HD13	1.81	0.62
1:A:343:LEU:O	1:A:343:LEU:HD23	2.00	0.62
1:A:339:ASP:O	1:A:343:LEU:HB2	2.01	0.61
1:A:383:ASP:O	1:A:387:LYS:HG3	2.00	0.61
1:A:385:PHE:C	1:A:385:PHE:CD1	2.77	0.61
1:A:277:LEU:CA	1:B:277:LEU:HD23	2.31	0.61
1:B:391:GLU:O	1:B:395:LEU:HD12	2.00	0.61
1:A:268:LYS:HG2	1:A:272:GLU:CD	2.27	0.60
1:B:396:LYS:O	1:B:399:ILE:HG22	2.01	0.60
1:B:382:MET:SD	1:B:382:MET:O	2.61	0.59
1:A:393:GLU:O	1:A:397:GLU:HG3	2.02	0.59
1:A:357:VAL:O	1:A:361:THR:HG23	2.03	0.59
1:B:371:LEU:O	1:B:371:LEU:HD23	2.02	0.59
1:B:343:LEU:HD22	1:B:347:GLU:CD	2.28	0.58
1:B:309:ARG:HH11	1:B:309:ARG:HG3	1.69	0.58
1:B:253:GLU:OE1	1:B:256:VAL:HG22	2.04	0.58
1:A:295:GLN:HG2	1:B:294:LEU:HD13	1.84	0.58
1:B:275:GLU:O	1:B:278:GLU:HB2	2.03	0.58
1:A:270:LEU:HD11	1:B:269:GLN:CB	2.24	0.58
1:A:332:GLN:O	1:A:336:GLN:HB2	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ASP:O	1:B:265:SER:HB3	2.03	0.57
1:A:354:ASP:O	1:A:358:GLU:HG3	2.04	0.57
1:B:330:SER:O	1:B:334:ASN:HB2	2.04	0.57
1:B:263:THR:HA	1:B:266:LEU:HD12	1.87	0.57
1:A:298:ASN:ND2	1:B:297:ARG:HB3	2.18	0.57
1:A:343:LEU:HG	1:B:343:LEU:HG	1.87	0.57
1:A:277:LEU:HA	1:B:277:LEU:CD2	2.35	0.56
1:B:299:VAL:HA	1:B:302:GLN:CG	2.36	0.56
1:B:353:LYS:HB2	1:B:353:LYS:NZ	2.22	0.55
1:B:335:GLN:O	1:B:339:ASP:HB2	2.06	0.55
1:A:314:THR:O	1:A:316:GLN:N	2.39	0.55
1:A:344:GLY:HA2	1:A:347:GLU:HG2	1.89	0.55
1:A:341:ARG:HB2	1:A:341:ARG:NH1	2.22	0.54
1:A:277:LEU:HG	1:B:277:LEU:HD23	1.89	0.54
1:A:281:GLY:HA2	1:B:280:VAL:HG11	1.89	0.54
1:A:372:GLU:O	1:A:376:LEU:HG	2.08	0.54
1:B:380:GLU:O	1:B:383:ASP:HB3	2.08	0.54
1:A:274:GLN:CG	1:B:273:ASN:ND2	2.71	0.53
1:B:406:ARG:HG2	1:B:406:ARG:NH1	2.19	0.53
1:A:331:GLN:HA	1:A:334:ASN:HD22	1.73	0.53
1:B:303:LYS:O	1:B:306:GLY:N	2.38	0.53
1:B:343:LEU:O	1:B:347:GLU:HG3	2.07	0.53
1:A:385:PHE:C	1:A:385:PHE:HD1	2.16	0.53
1:A:405:GLN:C	1:A:406:ARG:HD3	2.34	0.53
1:B:298:ASN:O	1:B:302:GLN:HG2	2.09	0.53
1:A:402:TYR:C	1:A:404:ALA:N	2.66	0.53
1:B:255:GLU:OE1	1:B:259:LEU:HD11	2.09	0.53
1:A:268:LYS:O	1:A:272:GLU:HG3	2.09	0.53
1:B:346:LEU:HD23	1:B:346:LEU:C	2.34	0.53
1:B:279:ILE:O	1:B:283:MET:HG3	2.08	0.52
1:B:272:GLU:O	1:B:275:GLU:N	2.41	0.52
1:B:258:ASP:O	1:B:262:ASP:HB2	2.09	0.52
1:A:275:GLU:O	1:A:279:ILE:HG13	2.09	0.52
1:A:291:VAL:HG12	1:A:292:ASP:N	2.25	0.52
1:A:338:LEU:HD23	1:A:341:ARG:HH22	1.74	0.52
1:A:367:LEU:O	1:A:371:LEU:HB2	2.10	0.52
1:B:282:ASN:O	1:B:283:MET:C	2.52	0.52
1:B:262:ASP:OD1	1:B:266:LEU:HD11	2.10	0.51
1:A:367:LEU:HD21	1:B:368:ARG:HE	1.75	0.51
1:B:255:GLU:HG2	1:B:259:LEU:HG	1.93	0.50
1:A:382:MET:O	1:A:386:GLU:HG3	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:LEU:O	1:B:284:LEU:HD23	2.11	0.50
1:A:268:LYS:HB2	1:A:268:LYS:HZ3	1.77	0.50
1:B:373:ASN:HB3	1:B:377:LYS:NZ	2.27	0.50
1:B:299:VAL:HA	1:B:302:GLN:HB2	1.94	0.50
1:A:256:VAL:O	1:A:260:LYS:HG3	2.12	0.50
1:A:284:LEU:HD22	1:B:283:MET:HB2	1.94	0.49
1:A:291:VAL:O	1:A:292:ASP:C	2.53	0.49
1:B:372:GLU:O	1:B:376:LEU:HG	2.13	0.49
1:B:406:ARG:HH11	1:B:406:ARG:CG	2.18	0.49
1:A:366:ILE:O	1:A:370:GLU:HG3	2.12	0.49
1:B:287:GLU:O	1:B:291:VAL:HG23	2.12	0.49
1:B:323:ASP:O	1:B:327:LYS:HG3	2.13	0.49
1:A:330:SER:O	1:A:333:GLN:HB2	2.12	0.49
1:A:360:LEU:HD22	1:B:364:ILE:CD1	2.43	0.49
1:A:326:LEU:HD23	1:B:326:LEU:HD23	1.95	0.48
1:A:395:LEU:O	1:A:396:LYS:C	2.56	0.48
1:B:328:ARG:HA	1:B:331:GLN:OE1	2.13	0.48
1:A:269:GLN:HB3	1:B:270:LEU:HD11	1.95	0.48
1:A:358:GLU:O	1:A:362:GLU:HG2	2.13	0.48
1:A:402:TYR:C	1:A:404:ALA:H	2.22	0.48
1:B:389:SER:O	1:B:392:ASN:HB3	2.14	0.48
1:B:324:GLN:HE21	1:B:327:LYS:NZ	2.12	0.48
1:A:341:ARG:CB	1:A:341:ARG:HH11	2.26	0.48
1:A:380:GLU:O	1:A:383:ASP:N	2.47	0.48
1:B:365:GLY:O	1:B:369:LYS:HG3	2.13	0.48
1:A:279:ILE:O	1:A:282:ASN:N	2.45	0.47
1:B:362:GLU:O	1:B:366:ILE:HG13	2.14	0.47
1:B:264:GLU:HB3	1:B:268:LYS:NZ	2.29	0.47
1:A:326:LEU:HD23	1:B:326:LEU:CD2	2.44	0.47
1:A:401:HIS:O	1:A:404:ALA:HB3	2.15	0.47
1:B:282:ASN:O	1:B:285:ARG:N	2.48	0.47
1:A:311:GLU:CB	1:B:312:LEU:HD11	2.44	0.47
1:B:262:ASP:O	1:B:266:LEU:HG	2.14	0.47
1:B:302:GLN:HE21	1:B:302:GLN:HA	1.81	0.46
1:B:354:ASP:O	1:B:358:GLU:HG3	2.15	0.46
1:A:314:THR:C	1:A:316:GLN:H	2.24	0.46
1:B:252:LYS:HE3	1:B:252:LYS:HA	1.98	0.46
1:A:325:LEU:HA	1:A:328:ARG:HG3	1.97	0.46
1:B:299:VAL:O	1:B:302:GLN:HB2	2.16	0.46
1:A:305:ILE:O	1:A:305:ILE:HG22	2.16	0.45
1:A:402:TYR:O	1:A:404:ALA:N	2.48	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:GLU:O	1:B:289:GLY:N	2.48	0.45
1:B:352:GLU:C	1:B:354:ASP:H	2.24	0.45
1:A:348:ALA:HA	1:A:351:LYS:HE2	1.96	0.45
1:A:295:GLN:HE21	1:B:294:LEU:CD1	2.27	0.45
1:A:356:MET:HE3	1:B:357:VAL:HG11	1.99	0.45
1:B:324:GLN:HE21	1:B:327:LYS:CE	2.30	0.45
1:A:292:ASP:O	1:A:295:GLN:HB2	2.16	0.45
1:B:272:GLU:C	1:B:274:GLN:N	2.74	0.45
1:B:373:ASN:HA	1:B:376:LEU:HG	1.99	0.45
1:A:314:THR:C	1:A:316:GLN:N	2.73	0.45
1:B:336:GLN:O	1:B:340:MET:HB2	2.17	0.45
1:B:303:LYS:O	1:B:304:GLU:C	2.60	0.45
1:B:377:LYS:O	1:B:381:ASN:HB2	2.16	0.44
1:A:318:ASN:HB3	1:B:319:LEU:CD1	2.45	0.44
1:B:286:GLU:C	1:B:289:GLY:H	2.25	0.44
1:B:266:LEU:HG	1:B:266:LEU:H	1.24	0.44
1:B:373:ASN:HB3	1:B:377:LYS:CE	2.47	0.44
1:A:314:THR:O	1:A:317:ARG:N	2.51	0.44
1:A:356:MET:HE3	1:B:357:VAL:CG1	2.47	0.44
1:B:299:VAL:CG1	1:B:302:GLN:HB2	2.48	0.43
1:B:299:VAL:HA	1:B:302:GLN:CB	2.49	0.43
1:A:347:GLU:N	1:B:346:LEU:HD11	2.34	0.43
1:A:309:ARG:HG3	1:A:309:ARG:HH11	1.84	0.43
1:B:256:VAL:HB	1:B:257:ALA:H	1.60	0.42
1:B:312:LEU:CD2	1:B:312:LEU:O	2.67	0.42
1:A:255:GLU:C	1:A:257:ALA:N	2.77	0.42
1:B:320:GLU:HA	1:B:320:GLU:OE1	2.19	0.42
1:B:324:GLN:NE2	1:B:327:LYS:NZ	2.67	0.42
1:B:352:GLU:C	1:B:354:ASP:N	2.73	0.42
1:B:406:ARG:NH1	1:B:406:ARG:CG	2.80	0.42
1:A:346:LEU:HB3	1:B:346:LEU:CD1	2.50	0.42
1:A:377:LYS:C	1:A:379:ALA:H	2.27	0.42
1:B:267:GLN:O	1:B:270:LEU:HB3	2.20	0.42
1:A:341:ARG:NH1	1:A:341:ARG:CB	2.82	0.42
1:B:393:GLU:O	1:B:394:ASN:C	2.63	0.42
1:A:338:LEU:O	1:A:342:LYS:HB2	2.19	0.42
1:B:393:GLU:C	1:B:395:LEU:N	2.77	0.42
1:A:282:ASN:ND2	1:A:285:ARG:HH22	2.18	0.41
1:A:336:GLN:HE21	1:A:336:GLN:HA	1.85	0.41
1:A:377:LYS:C	1:A:379:ALA:N	2.76	0.41
1:B:368:ARG:O	1:B:372:GLU:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:ASN:O	1:B:277:LEU:HB2	2.19	0.41
1:A:336:GLN:HE21	1:A:336:GLN:CA	2.34	0.41
1:A:336:GLN:HA	1:A:336:GLN:NE2	2.36	0.41
1:A:273:ASN:OD1	1:A:273:ASN:C	2.64	0.41
1:A:388:LEU:HD13	1:B:388:LEU:CG	2.46	0.41
1:B:259:LEU:O	1:B:263:THR:HG23	2.21	0.41
1:A:330:SER:HA	1:A:333:GLN:NE2	2.36	0.40
1:A:388:LEU:HD11	1:B:389:SER:HA	2.02	0.40
1:B:338:LEU:CD1	1:B:342:LYS:NZ	2.84	0.40
1:B:257:ALA:HB1	1:B:261:GLN:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	156/167 (93%)	140 (90%)	14 (9%)	2 (1%)	9	35
1	B	156/167 (93%)	138 (88%)	15 (10%)	3 (2%)	6	28
All	All	312/334 (93%)	278 (89%)	29 (9%)	5 (2%)	7	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	256	VAL
1	B	405	GLN
1	A	315	ALA
1	A	403	ARG
1	B	252	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	A	142/149 (95%)	127 (89%)	15 (11%)	6	24
1	B	142/149 (95%)	121 (85%)	21 (15%)	3	13
All	All	284/298 (95%)	248 (87%)	36 (13%)	4	18

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	ASP
1	A	261	GLN
1	A	263	THR
1	A	264	GLU
1	A	267	GLN
1	A	275	GLU
1	A	277	LEU
1	A	278	GLU
1	A	297	ARG
1	A	352	GLU
1	A	354	ASP
1	A	356	MET
1	A	371	LEU
1	A	385	PHE
1	A	388	LEU
1	B	250	GLU
1	B	252	LYS
1	B	253	GLU
1	B	256	VAL
1	B	258	ASP
1	B	266	LEU
1	B	283	MET
1	B	284	LEU
1	B	302	GLN
1	B	312	LEU
1	B	320	GLU
1	B	343	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	350	LEU
1	B	353	LYS
1	B	354	ASP
1	B	368	ARG
1	B	389	SER
1	B	398	LYS
1	B	399	ILE
1	B	405	GLN
1	B	407	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	282	ASN
1	A	295	GLN
1	A	298	ASN
1	A	331	GLN
1	A	333	GLN
1	A	334	ASN
1	A	335	GLN
1	B	261	GLN
1	B	267	GLN
1	B	273	ASN
1	B	302	GLN
1	B	324	GLN
1	B	331	GLN
1	B	332	GLN
1	B	392	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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 [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	158/167 (94%)	0.11	3 (1%) 66 48	49, 107, 171, 205	0
1	B	158/167 (94%)	0.28	7 (4%) 39 25	36, 114, 185, 247	0
All	All	316/334 (94%)	0.19	10 (3%) 50 34	36, 109, 176, 247	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	276	GLU	3.9
1	B	322	ALA	3.2
1	A	267	GLN	3.2
1	B	259	LEU	3.0
1	B	342	LYS	3.0
1	B	325	LEU	2.9
1	B	338	LEU	2.2
1	A	256	VAL	2.2
1	B	263	THR	2.1
1	B	370	GLU	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.