



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:42 PM UTC

PDB ID : 3K8P / pdb_00003k8p
Title : Structural basis for vesicle tethering by the Dsl1 complex
Authors : Ren, Y.; Jeffrey, P.D.; Hughson, F.M.
Deposited on : 2009-10-14
Resolution : 2.60 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

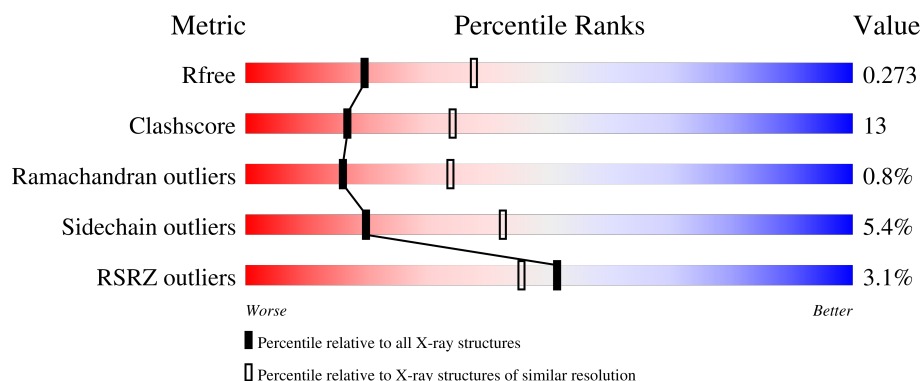
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	C	357	
2	D	709	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7376 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 Dsl1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	295	Total	C	N	O	S	Se	0	0	0
			2464	1594	404	458	2	6			

There are 2 discrepancies between the modelled and reference sequences:

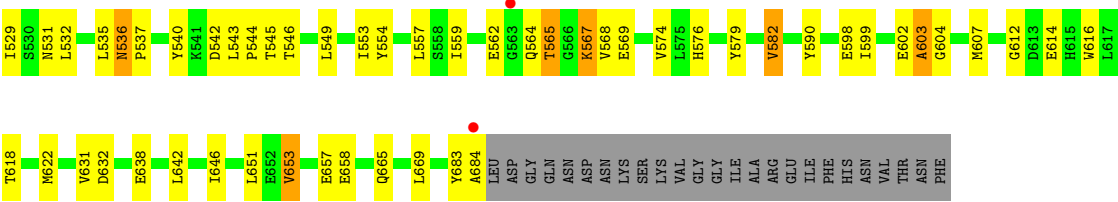
Chain	Residue	Modelled	Actual	Comment	Reference
C	330	GLY	-	expression tag	UNP Q6CUS2
C	331	SER	-	expression tag	UNP Q6CUS2

- Molecule 2 is a protein called Protein transport protein SEC39.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	594	Total	C	N	O	S	Se	0	0	0
			4909	3182	775	931	7	14			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	3	Total	O	0	0
			3	3		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.02Å 90.82Å 213.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.20 – 2.60 31.20 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.5 (31.20-2.60) 97.8 (31.20-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.08 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.205 , 0.271 0.213 , 0.273	Depositor DCC
R_{free} test set	2212 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7376	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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	C	0.54	0/2503	0.87	2/3376 (0.1%)
2	D	0.50	0/4998	0.84	7/6724 (0.1%)
All	All	0.51	0/7501	0.85	9/10100 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	269	ALA	N-CA-C	-7.02	104.72	113.28
1	C	450	ARG	N-CA-C	-6.95	95.99	110.80
2	D	653	VAL	CB-CA-C	-6.54	103.67	111.65
2	D	536	ASN	CA-C-N	5.86	125.56	119.82
2	D	536	ASN	C-N-CA	5.86	125.56	119.82
2	D	653	VAL	N-CA-C	5.41	117.41	112.43
2	D	138	THR	CA-C-N	5.29	124.90	119.56
2	D	138	THR	C-N-CA	5.29	124.90	119.56
1	C	578	VAL	N-CA-C	5.13	115.28	110.30

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	C	2464	0	2516	48	0
2	D	4909	0	4886	143	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	3	0	0	0	0
All	All	7376	0	7402	189	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 13.

All (189) 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)
2:D:435:TYR:HB2	2:D:473:MSE:HE2	1.42	0.97
2:D:316:GLU:HG3	2:D:317:GLN:H	1.32	0.94
2:D:348:THR:HG22	2:D:349:GLN:HG3	1.57	0.87
2:D:546:THR:HG21	2:D:576:HIS:CE1	2.11	0.86
2:D:603:ALA:HB1	2:D:607:MSE:HG3	1.57	0.84
2:D:500:ASN:H	2:D:531:ASN:HD21	1.22	0.84
2:D:132:ASN:HD21	2:D:182:ILE:H	1.27	0.82
1:C:467:ALA:O	1:C:471:MSE:HG3	1.82	0.79
2:D:435:TYR:HB2	2:D:473:MSE:CE	2.13	0.78
2:D:435:TYR:CB	2:D:473:MSE:HE2	2.16	0.73
2:D:540:TYR:O	2:D:576:HIS:HD2	1.72	0.72
2:D:590:TYR:HD1	2:D:646:ILE:HD11	1.54	0.72
2:D:565:THR:O	2:D:569:GLU:HG3	1.89	0.72
2:D:622:MSE:SE	2:D:646:ILE:HD13	2.40	0.71
2:D:360:SER:HB2	2:D:409:ILE:HD11	1.73	0.71
2:D:117:LEU:HD11	2:D:123:TRP:HA	1.72	0.71
2:D:590:TYR:CD1	2:D:646:ILE:HD11	2.26	0.71
2:D:387:ILE:HG23	2:D:399:MSE:HE2	1.73	0.70
1:C:654:ASP:OD1	1:C:678:ARG:NH2	2.25	0.69
2:D:192:GLU:O	2:D:196:ILE:HG23	1.91	0.69
2:D:542:ASP:OD1	2:D:545:THR:HG23	1.94	0.68
2:D:101:TYR:CE2	2:D:104:LEU:HD22	2.28	0.68
2:D:191:SER:O	2:D:195:LYS:HG3	1.94	0.67
1:C:439:THR:HG22	1:C:443:GLN:HE21	1.60	0.67
2:D:108:ILE:HG13	2:D:109:SER:N	2.10	0.67
2:D:33:SER:O	2:D:37:GLU:HG3	1.95	0.66
2:D:562:GLU:OE2	2:D:564:GLN:HG3	1.96	0.66
2:D:132:ASN:ND2	2:D:182:ILE:H	1.92	0.66
1:C:511:LEU:HD11	1:C:565:ILE:HG23	1.78	0.66
2:D:30:GLY:HA3	2:D:31:SER:O	1.95	0.66
2:D:316:GLU:HG3	2:D:317:GLN:N	2.09	0.66
1:C:644:TYR:OH	1:C:676:GLU:OE2	2.13	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:315:GLU:HG2	2:D:316:GLU:N	2.12	0.65
2:D:431:ASN:O	2:D:473:MSE:HE1	1.97	0.65
2:D:117:LEU:HD11	2:D:123:TRP:CA	2.26	0.64
1:C:636:LEU:HD23	1:C:669:THR:HG22	1.79	0.63
1:C:639:ILE:HA	1:C:642:MSE:HE3	1.81	0.63
1:C:618:TYR:CZ	1:C:622:ARG:HD2	2.34	0.62
1:C:431:VAL:HG11	1:C:488:TYR:CD2	2.34	0.62
2:D:500:ASN:H	2:D:531:ASN:ND2	1.98	0.60
2:D:590:TYR:HD1	2:D:646:ILE:CD1	2.15	0.60
2:D:175:ARG:NH2	2:D:176:LEU:HD21	2.16	0.60
2:D:134:MSE:O	2:D:135:ILE:HD13	2.02	0.59
2:D:387:ILE:CG2	2:D:399:MSE:HE2	2.33	0.59
1:C:450:ARG:O	1:C:452:LYS:N	2.35	0.58
2:D:603:ALA:CB	2:D:607:MSE:HG3	2.33	0.58
2:D:514:LYS:HE2	2:D:516:SER:OG	2.03	0.58
2:D:590:TYR:CZ	2:D:642:LEU:HD22	2.38	0.58
2:D:567:LYS:HZ1	2:D:614:GLU:CD	2.11	0.58
2:D:546:THR:HG21	2:D:576:HIS:HE1	1.67	0.57
2:D:316:GLU:HG2	2:D:318:LYS:HD2	1.87	0.57
2:D:112:LEU:O	2:D:115:LYS:HE3	2.03	0.57
2:D:316:GLU:CG	2:D:317:GLN:H	2.10	0.57
2:D:53:LEU:HD11	2:D:56:ARG:NH2	2.20	0.56
2:D:105:GLN:HA	2:D:108:ILE:HG12	1.86	0.56
2:D:160:GLY:O	2:D:164:GLY:N	2.38	0.56
2:D:564:GLN:O	2:D:568:VAL:HG23	2.06	0.56
2:D:638:GLU:OE1	2:D:684:ALA:HB1	2.05	0.55
2:D:554:TYR:HA	2:D:559:ILE:HD12	1.87	0.55
2:D:108:ILE:HG13	2:D:109:SER:H	1.70	0.55
2:D:567:LYS:NZ	2:D:614:GLU:OE1	2.40	0.55
2:D:238:LYS:HG3	2:D:239:GLN:HE21	1.72	0.55
2:D:315:GLU:CG	2:D:316:GLU:H	2.18	0.54
1:C:425:ILE:HG13	1:C:426:GLN:N	2.22	0.54
2:D:101:TYR:HE2	2:D:104:LEU:HD22	1.73	0.54
2:D:683:TYR:O	2:D:684:ALA:HB3	2.08	0.54
2:D:315:GLU:HG2	2:D:316:GLU:H	1.72	0.54
2:D:529:ILE:HA	2:D:532:LEU:HD12	1.89	0.53
2:D:318:LYS:HG2	2:D:345:PHE:CE2	2.43	0.53
2:D:132:ASN:HD21	2:D:182:ILE:N	2.01	0.53
2:D:60:GLU:O	2:D:61:GLU:HB2	2.08	0.53
2:D:219:ALA:HB3	2:D:220:PRO:HD3	1.91	0.52
2:D:155:SER:OG	2:D:157:LYS:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:52:LEU:HD13	2:D:123:TRP:CH2	2.45	0.52
2:D:454:ARG:HG2	2:D:492:ASP:OD2	2.10	0.52
2:D:60:GLU:HG2	2:D:153:VAL:HG11	1.91	0.52
2:D:124:LEU:O	2:D:128:ILE:HG13	2.11	0.51
2:D:134:MSE:C	2:D:135:ILE:HD13	2.36	0.51
2:D:616:TRP:CZ2	2:D:658:GLU:HG3	2.46	0.51
2:D:61:GLU:O	2:D:62:VAL:C	2.54	0.51
2:D:459:MSE:CE	2:D:488:LEU:HD22	2.42	0.50
1:C:573:ILE:O	1:C:577:LEU:HB3	2.11	0.50
1:C:431:VAL:CG1	1:C:488:TYR:CD2	2.95	0.50
2:D:57:GLU:C	2:D:59:GLU:H	2.20	0.50
2:D:366:GLU:HG3	2:D:376:PHE:CE1	2.46	0.49
2:D:490:ILE:HD13	2:D:553:ILE:HG12	1.95	0.49
2:D:360:SER:HB3	2:D:405:SER:OG	2.12	0.49
1:C:683:GLU:O	1:C:684:ALA:C	2.56	0.49
2:D:622:MSE:SE	2:D:646:ILE:CD1	3.11	0.49
1:C:471:MSE:HG2	2:D:651:LEU:CB	2.43	0.48
2:D:359:PHE:HE2	2:D:384:VAL:CG1	2.26	0.48
1:C:511:LEU:HD11	1:C:565:ILE:CG2	2.43	0.48
1:C:497:LEU:HD22	1:C:500:MSE:HE2	1.96	0.48
2:D:112:LEU:O	2:D:115:LYS:HB2	2.13	0.48
1:C:366:GLN:HA	1:C:366:GLN:OE1	2.14	0.48
1:C:441:PHE:CE1	1:C:461:PHE:CD1	3.02	0.48
2:D:631:VAL:O	2:D:632:ASP:HB2	2.12	0.48
1:C:523:ASN:OD1	1:C:581:ASN:ND2	2.47	0.48
2:D:579:TYR:HA	2:D:582:VAL:HB	1.95	0.48
2:D:30:GLY:CA	2:D:31:SER:HB2	2.44	0.47
2:D:143:SER:HA	2:D:146:TRP:CE2	2.50	0.47
2:D:345:PHE:O	2:D:348:THR:HB	2.14	0.47
2:D:459:MSE:HE1	2:D:488:LEU:HD22	1.97	0.47
2:D:562:GLU:HG2	2:D:562:GLU:O	2.14	0.47
2:D:658:GLU:HA	2:D:658:GLU:OE1	2.15	0.47
2:D:665:GLN:HE21	2:D:669:LEU:HD11	1.80	0.47
2:D:514:LYS:H	2:D:517:ASN:ND2	2.12	0.47
2:D:562:GLU:C	2:D:564:GLN:N	2.72	0.47
2:D:612:GLY:HA3	2:D:653:VAL:O	2.14	0.47
1:C:613:ASN:O	1:C:619:ARG:NH1	2.49	0.46
2:D:522:ARG:O	2:D:522:ARG:HG2	2.16	0.46
2:D:168:PRO:HG3	2:D:220:PRO:HB2	1.97	0.46
2:D:126:GLU:O	2:D:130:ILE:HG13	2.14	0.46
2:D:315:GLU:CG	2:D:316:GLU:N	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:101:TYR:O	2:D:101:TYR:HD2	1.99	0.46
2:D:350:GLU:OE1	2:D:358:HIS:HD2	1.99	0.46
1:C:483:TYR:CD1	1:C:503:ASN:ND2	2.84	0.46
2:D:140:LEU:O	2:D:141:LEU:C	2.58	0.46
2:D:117:LEU:HD11	2:D:123:TRP:CB	2.46	0.46
1:C:358:GLU:HG2	1:C:429:VAL:HG12	1.98	0.45
1:C:582:ILE:HD13	1:C:596:LEU:HD22	1.97	0.45
1:C:558:TYR:HD1	1:C:566:LEU:HD11	1.82	0.45
2:D:562:GLU:C	2:D:564:GLN:H	2.24	0.45
2:D:562:GLU:H	2:D:562:GLU:CD	2.24	0.45
2:D:598:GLU:O	2:D:599:ILE:C	2.57	0.45
1:C:562:ASP:OD1	1:C:564:THR:HB	2.16	0.45
1:C:468:PHE:CE2	1:C:472:VAL:HG21	2.52	0.45
2:D:106:GLU:O	2:D:110:LYS:HB2	2.16	0.45
1:C:361:GLU:O	1:C:429:VAL:HG23	2.17	0.45
1:C:579:ILE:HD13	1:C:624:LYS:HD3	1.97	0.44
1:C:627:ILE:HD13	1:C:647:GLU:O	2.16	0.44
2:D:31:SER:CB	2:D:34:LYS:HG2	2.47	0.44
2:D:351:GLU:HG2	2:D:352:GLU:N	2.32	0.44
2:D:407:LEU:CD1	2:D:434:ILE:HD12	2.47	0.44
1:C:446:ASP:C	1:C:448:ILE:H	2.24	0.44
1:C:431:VAL:CG1	1:C:488:TYR:HD2	2.30	0.44
2:D:435:TYR:CA	2:D:473:MSE:HE2	2.47	0.44
1:C:558:TYR:CD1	1:C:566:LEU:HD11	2.53	0.44
2:D:52:LEU:HD13	2:D:123:TRP:HH2	1.80	0.44
1:C:343:MSE:HE1	1:C:441:PHE:CD2	2.53	0.44
2:D:490:ILE:HG13	2:D:491:SER:N	2.31	0.44
2:D:536:ASN:HA	2:D:537:PRO:HD3	1.80	0.44
2:D:543:LEU:N	2:D:544:PRO:CD	2.80	0.44
1:C:524:ASP:HB3	1:C:540:ILE:HD13	2.00	0.44
2:D:488:LEU:HD23	2:D:488:LEU:HA	1.75	0.44
1:C:625:LEU:HD23	1:C:625:LEU:HA	1.83	0.43
1:C:640:LEU:HG	1:C:644:TYR:CE2	2.53	0.43
1:C:471:MSE:HG2	2:D:651:LEU:HB3	1.99	0.43
2:D:366:GLU:HG3	2:D:376:PHE:CZ	2.54	0.43
1:C:518:ILE:HD13	1:C:573:ILE:HD11	1.99	0.43
1:C:347:ARG:HA	1:C:347:ARG:NE	2.34	0.43
1:C:636:LEU:HD12	1:C:636:LEU:HA	1.79	0.43
1:C:636:LEU:HD21	1:C:670:ARG:HA	2.01	0.43
2:D:117:LEU:HD11	2:D:123:TRP:HB2	2.01	0.43
2:D:263:VAL:O	2:D:264:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:602:GLU:C	2:D:604:GLY:N	2.75	0.42
1:C:453:VAL:HG12	1:C:457:TYR:HB2	2.00	0.42
2:D:192:GLU:HA	2:D:195:LYS:HB2	2.01	0.42
1:C:340:PHE:HE1	1:C:453:VAL:HG13	1.85	0.42
2:D:56:ARG:NH1	2:D:148:THR:C	2.77	0.42
2:D:101:TYR:O	2:D:104:LEU:HB2	2.19	0.42
2:D:542:ASP:CG	2:D:545:THR:HG23	2.45	0.42
1:C:519:TYR:CZ	1:C:523:ASN:ND2	2.88	0.42
2:D:249:TYR:O	2:D:252:PHE:HB3	2.20	0.42
2:D:53:LEU:HD11	2:D:56:ARG:HH21	1.84	0.42
2:D:143:SER:O	2:D:147:GLU:HB2	2.20	0.42
2:D:255:LEU:HD23	2:D:255:LEU:HA	1.81	0.42
1:C:338:LEU:C	1:C:338:LEU:HD23	2.45	0.41
1:C:640:LEU:HD12	1:C:640:LEU:HA	1.82	0.41
2:D:39:LEU:HA	2:D:39:LEU:HD12	1.82	0.41
2:D:46:LEU:CD1	2:D:135:ILE:HD11	2.50	0.41
2:D:57:GLU:C	2:D:59:GLU:N	2.77	0.41
2:D:213:VAL:HG12	2:D:214:ILE:HD13	2.02	0.41
2:D:549:LEU:O	2:D:553:ILE:HG13	2.20	0.41
2:D:218:LEU:HD11	2:D:231:PHE:CE1	2.55	0.41
2:D:456:GLU:HA	2:D:457:PRO:HD3	1.94	0.41
2:D:261:LYS:HB3	2:D:261:LYS:HE2	1.78	0.41
2:D:30:GLY:HA2	2:D:31:SER:HB2	2.03	0.41
2:D:574:VAL:HG13	2:D:618:THR:HG21	2.01	0.41
2:D:683:TYR:O	2:D:684:ALA:CB	2.68	0.41
2:D:55:LEU:HD23	2:D:55:LEU:HA	1.80	0.41
2:D:213:VAL:O	2:D:217:GLU:HB2	2.20	0.41
1:C:341:GLU:O	1:C:345:GLN:HG3	2.21	0.41
2:D:411:LEU:HG	2:D:419:ILE:HD13	2.03	0.41
2:D:500:ASN:CG	2:D:535:LEU:HD11	2.46	0.41
2:D:411:LEU:HG	2:D:419:ILE:CD1	2.51	0.40
2:D:56:ARG:HH12	2:D:148:THR:C	2.29	0.40
2:D:311:GLU:O	2:D:312:ILE:HD13	2.21	0.40
2:D:522:ARG:NH1	2:D:557:LEU:O	2.55	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	C	291/357 (82%)	278 (96%)	11 (4%)	2 (1%)	18	38
2	D	584/709 (82%)	548 (94%)	31 (5%)	5 (1%)	14	30
All	All	875/1066 (82%)	826 (94%)	42 (5%)	7 (1%)	16	34

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	448	ILE
1	C	450	ARG
2	D	316	GLU
2	D	31	SER
2	D	61	GLU
2	D	151	SER
2	D	603	ALA

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	C	281/330 (85%)	270 (96%)	11 (4%)	28	55
2	D	555/641 (87%)	521 (94%)	34 (6%)	17	37
All	All	836/971 (86%)	791 (95%)	45 (5%)	20	42

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	363	VAL
1	C	425	ILE
1	C	448	ILE
1	C	458	LEU
1	C	491	THR
1	C	501	GLU
1	C	511	LEU
1	C	570	ILE
1	C	623	GLU
1	C	650	LEU
1	C	652	GLU
2	D	38	ILE
2	D	46	LEU
2	D	58	LEU
2	D	117	LEU
2	D	118	GLU
2	D	122	GLU
2	D	125	ARG
2	D	140	LEU
2	D	141	LEU
2	D	147	GLU
2	D	148	THR
2	D	183	ASN
2	D	193	LEU
2	D	196	ILE
2	D	223	SER
2	D	246	ASP
2	D	263	VAL
2	D	264	LYS
2	D	268	GLU
2	D	272	LYS
2	D	303	SER
2	D	311	GLU
2	D	323	LEU
2	D	348	THR
2	D	351	GLU
2	D	384	VAL
2	D	427	ASP
2	D	456	GLU
2	D	473	MSE
2	D	524	CYS
2	D	565	THR
2	D	567	LYS

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Mol	Chain	Res	Type
2	D	582	VAL
2	D	657	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	360	HIS
1	C	443	GLN
1	C	532	ASN
1	C	563	ASN
1	C	575	HIS
1	C	620	HIS
2	D	114	ASN
2	D	132	ASN
2	D	239	GLN
2	D	276	ASN
2	D	368	ASN
2	D	430	ASN
2	D	444	HIS
2	D	467	GLN
2	D	517	ASN
2	D	531	ASN
2	D	576	HIS
2	D	665	GLN

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

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	C	289/357 (80%)	-0.23	9 (3%)	51	45	30, 51, 106, 149	0
2	D	580/709 (81%)	-0.02	18 (3%)	51	45	35, 59, 102, 145	0
All	All	869/1066 (81%)	-0.09	27 (3%)	51	45	30, 56, 103, 149	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	334	ILE	4.6
2	D	62	VAL	4.5
2	D	502	ASN	3.6
1	C	443	GLN	3.6
1	C	335	TYR	3.4
2	D	684	ALA	3.4
2	D	101	TYR	2.9
2	D	563	GLY	2.9
2	D	264	LYS	2.8
1	C	424	PRO	2.8
2	D	177	HIS	2.6
1	C	448	ILE	2.5
2	D	198	PHE	2.4
2	D	38	ILE	2.3
2	D	133	GLU	2.3
1	C	425	ILE	2.3
1	C	338	LEU	2.3
2	D	31	SER	2.2
2	D	199	ASP	2.2
2	D	61	GLU	2.1
2	D	211	ALA	2.1
2	D	512	ALA	2.1
2	D	39	LEU	2.1
1	C	451	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	107	PHE	2.1
2	D	268	GLU	2.0
1	C	432	GLN	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.