



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:26 AM UTC

PDB ID : 2FU3 / pdb_00002fu3
Title : Crystal structure of gephyrin E-domain
Authors : Kim, E.Y.; Schindelin, H.
Deposited on : 2006-01-25
Resolution : 2.70 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

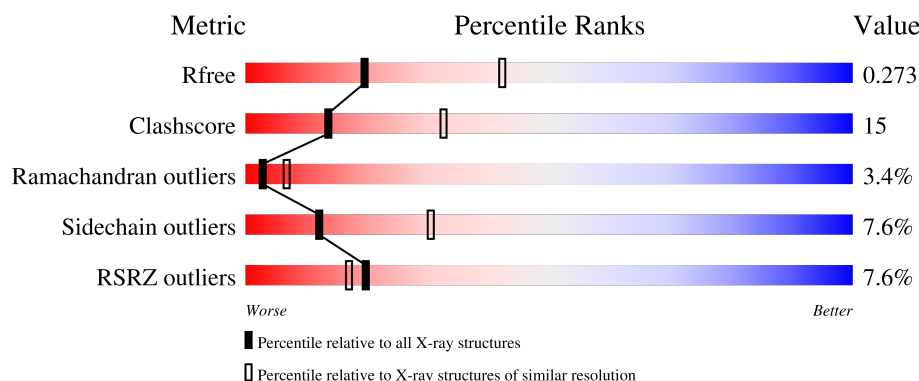
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	419	6% 66% 25% 5%
1	B	419	9% 66% 26% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6257 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 gephyrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3054	1930	531	572	21			
1	B	419	Total	C	N	O	S	0	0	0
			3137	1978	548	591	20			

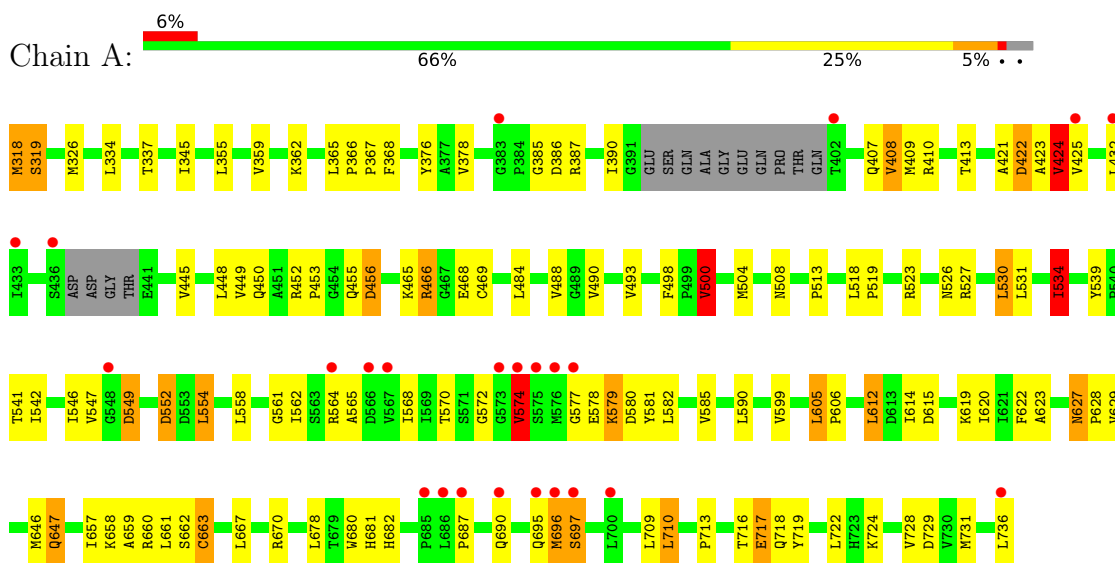
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	37	Total	O	0	0
			37	37		
2	B	29	Total	O	0	0
			29	29		

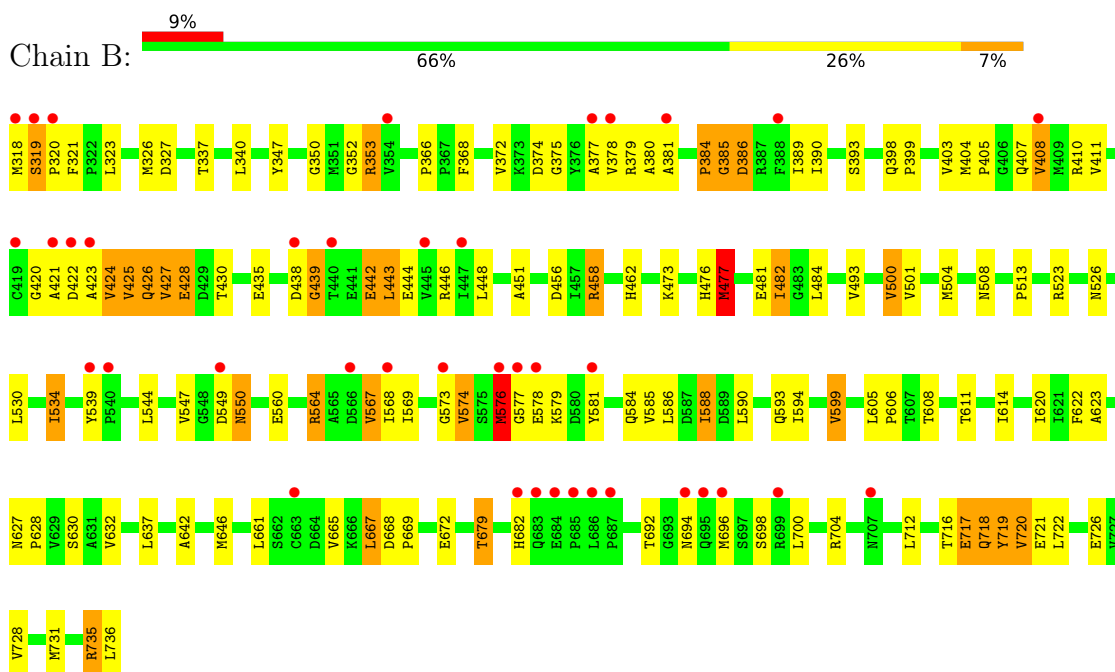
3 Residue-property plots

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: gephyrin



• Molecule 1: gephyrin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	108.82Å 156.19Å 51.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.70) 99.6 (20.00-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.202 , 0.273 0.209 , 0.273	Depositor DCC
R_{free} test set	1748 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	58.7	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 68.2	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	0.91	EDS
Total number of atoms	6257	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.08% 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	1.37	14/3112 (0.4%)	0.97	5/4233 (0.1%)
1	B	1.36	11/3198 (0.3%)	1.03	10/4355 (0.2%)
All	All	1.37	25/6310 (0.4%)	1.00	15/8588 (0.2%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	424	VAL	CA-CB	8.45	1.66	1.54
1	B	500	VAL	CA-CB	8.12	1.64	1.54
1	B	574	VAL	CA-CB	8.07	1.65	1.54
1	A	710	LEU	C-O	-7.25	1.15	1.23
1	A	534	ILE	CA-CB	7.15	1.63	1.54
1	B	569	ILE	CA-CB	-6.83	1.46	1.54
1	B	576	MET	CA-C	6.80	1.59	1.53
1	A	659	ALA	CA-CB	-6.76	1.42	1.53
1	A	500	VAL	CA-C	6.59	1.60	1.52
1	B	594	ILE	C-O	-6.44	1.17	1.24
1	A	530	LEU	C-O	-6.42	1.16	1.24
1	B	720	VAL	CA-CB	6.41	1.62	1.54
1	A	622	PHE	CA-C	-6.09	1.45	1.52
1	A	359	VAL	CA-CB	-5.87	1.47	1.54
1	A	574	VAL	CA-C	5.79	1.60	1.52
1	A	534	ILE	CB-CG1	-5.74	1.42	1.53
1	A	390	ILE	CA-CB	5.66	1.62	1.54
1	A	647	GLN	N-CA	5.50	1.52	1.46
1	B	473	LYS	CA-C	5.42	1.59	1.52
1	B	567	VAL	CA-CB	-5.42	1.47	1.54
1	B	622	PHE	CA-C	-5.40	1.46	1.52
1	B	577	GLY	N-CA	5.27	1.53	1.45
1	A	345	ILE	CA-CB	-5.19	1.47	1.54
1	B	642	ALA	C-O	-5.05	1.18	1.24
1	A	670	ARG	CA-C	5.05	1.59	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	422	ASP	N-CA-C	-7.18	100.69	110.68
1	B	588	ILE	N-CA-C	6.92	118.55	111.00
1	B	368	PHE	CA-C-N	-6.10	113.48	119.76
1	B	368	PHE	C-N-CA	-6.10	113.48	119.76
1	B	482	ILE	N-CA-C	-5.77	104.89	110.72
1	B	501	VAL	N-CA-C	5.63	115.96	107.80
1	A	574	VAL	N-CA-C	5.63	121.05	109.34
1	B	442	GLU	N-CA-C	5.38	116.90	110.44
1	A	448	LEU	N-CA-C	5.27	120.36	113.88
1	A	385	GLY	N-CA-C	5.26	117.22	110.96
1	B	380	ALA	N-CA-C	-5.24	107.18	113.21
1	B	477	MET	N-CA-C	5.24	118.08	109.76
1	B	443	LEU	N-CA-C	5.14	121.74	110.80
1	A	500	VAL	N-CA-CB	5.10	116.09	110.53
1	A	663	CYS	N-CA-C	5.01	115.76	108.14

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	3054	0	3072	87	0
1	B	3137	0	3127	99	0
2	A	37	0	0	1	0
2	B	29	0	0	1	0
All	All	6257	0	6199	181	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 15.

All (181) 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:526:ASN:HD21	1:B:628:PRO:HA	1.40	0.86
1:A:362:LYS:O	1:A:466:ARG:HD2	1.76	0.86
1:A:449:VAL:HG12	1:A:450:GLN:H	1.41	0.85
1:A:627:ASN:HD21	1:A:695:GLN:HE21	1.22	0.84
1:B:424:VAL:O	1:B:425:VAL:HG23	1.81	0.79
1:A:378:VAL:HG21	1:A:425:VAL:HG21	1.66	0.76
1:B:718:GLN:O	1:B:719:TYR:C	2.33	0.72
1:B:534:ILE:CD1	1:B:539:TYR:HB2	2.19	0.71
1:B:627:ASN:HD22	1:B:630:SER:H	1.36	0.71
1:B:637:LEU:HD23	1:B:731:MET:HE1	1.73	0.70
1:A:629:VAL:HG21	1:A:695:GLN:HA	1.71	0.70
1:A:627:ASN:ND2	1:A:695:GLN:HE21	1.90	0.69
1:B:337:THR:HG23	1:B:646:MET:HE2	1.74	0.69
1:B:424:VAL:CG2	1:B:456:ASP:HB2	2.22	0.69
1:A:696:MET:HE3	1:B:462:HIS:CE1	2.28	0.69
1:B:423:ALA:O	1:B:424:VAL:HB	1.92	0.68
1:B:378:VAL:O	1:B:423:ALA:HA	1.95	0.66
1:B:504:MET:HE3	1:B:547:VAL:HG21	1.78	0.66
1:B:425:VAL:HG12	1:B:426:GLN:N	2.11	0.64
1:A:534:ILE:CD1	1:A:539:TYR:HB2	2.28	0.64
1:A:526:ASN:O	1:A:527:ARG:C	2.41	0.63
1:B:584:GLN:HG3	1:B:588:ILE:HD12	1.81	0.63
1:B:375:GLY:HA3	1:B:425:VAL:HB	1.81	0.62
1:B:379:ARG:HG2	1:B:421:ALA:HB2	1.80	0.62
1:B:620:ILE:HD11	1:B:646:MET:HE1	1.81	0.62
1:A:562:ILE:O	1:A:619:LYS:NZ	2.31	0.62
1:A:466:ARG:HH21	1:A:466:ARG:HG3	1.66	0.61
1:A:423:ALA:N	2:A:34:HOH:O	2.32	0.61
1:A:620:ILE:HD11	1:A:646:MET:HE1	1.82	0.61
1:B:534:ILE:HD12	1:B:539:TYR:HB2	1.83	0.60
1:A:562:ILE:N	1:A:568:ILE:HD11	2.17	0.59
1:B:442:GLU:O	1:B:444:GLU:N	2.32	0.59
1:B:513:PRO:HA	1:B:523:ARG:HD3	1.86	0.58
1:B:389:ILE:HD12	1:B:442:GLU:O	2.04	0.58
1:B:564:ARG:HG2	1:B:564:ARG:HH11	1.68	0.57
1:A:552:ASP:OD2	1:A:552:ASP:N	2.36	0.57
1:A:449:VAL:HG12	1:A:450:GLN:N	2.16	0.57
1:A:612:LEU:HD13	1:A:614:ILE:HD11	1.86	0.57
1:B:424:VAL:HG21	1:B:456:ASP:HB2	1.87	0.56
1:A:581:TYR:O	1:A:585:VAL:HG23	2.05	0.56
1:B:372:VAL:HB	1:B:456:ASP:HB3	1.86	0.56
1:B:735:ARG:HB2	1:B:735:ARG:HH11	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:ILE:HD12	1:A:539:TYR:HB2	1.87	0.55
1:A:500:VAL:HG22	1:A:565:ALA:HA	1.88	0.55
1:A:574:VAL:HA	1:A:579:LYS:HB2	1.87	0.54
1:A:696:MET:CE	1:B:462:HIS:CE1	2.89	0.54
1:A:680:TRP:CE2	1:A:687:PRO:HB3	2.42	0.54
1:A:605:LEU:HD13	1:A:605:LEU:C	2.32	0.54
1:A:424:VAL:HG13	1:A:425:VAL:H	1.73	0.54
1:B:347:TYR:O	1:B:482:ILE:HD12	2.09	0.53
1:A:376:TYR:HB3	1:A:408:VAL:HG13	1.91	0.53
1:B:379:ARG:C	1:B:381:ALA:H	2.17	0.53
1:B:573:GLY:HA2	1:B:579:LYS:HB3	1.90	0.53
1:B:323:LEU:HD21	1:B:605:LEU:HD11	1.90	0.52
1:B:526:ASN:ND2	1:B:628:PRO:HA	2.19	0.52
1:B:692:THR:HA	1:B:700:LEU:HD13	1.91	0.52
1:B:728:VAL:HG13	2:B:39:HOH:O	2.09	0.51
1:B:404:MET:HB3	1:B:405:PRO:HD2	1.93	0.51
1:B:398:GLN:OE1	1:B:399:PRO:HD2	2.11	0.51
1:B:679:THR:HB	1:B:704:ARG:HH22	1.75	0.51
1:B:716:THR:HG22	1:B:718:GLN:H	1.75	0.51
1:A:508:ASN:HD21	1:A:549:ASP:H	1.58	0.51
1:A:526:ASN:HD21	1:A:628:PRO:HA	1.76	0.51
1:B:477:MET:HG3	1:B:481:GLU:HB2	1.93	0.51
1:B:679:THR:HB	1:B:704:ARG:NH2	2.25	0.51
1:B:735:ARG:HH11	1:B:735:ARG:CG	2.24	0.50
1:A:542:ILE:HD13	1:A:564:ARG:HG2	1.92	0.50
1:B:377:ALA:HA	1:B:423:ALA:CB	2.41	0.50
1:A:513:PRO:HA	1:A:523:ARG:HD3	1.93	0.50
1:A:424:VAL:HG12	1:A:455:GLN:HE21	1.77	0.49
1:A:627:ASN:ND2	1:A:629:VAL:H	2.10	0.49
1:A:530:LEU:O	1:A:534:ILE:HG23	2.12	0.49
1:A:657:ILE:HD11	1:A:678:LEU:HD13	1.95	0.49
1:A:386:ASP:C	1:A:387:ARG:HG3	2.37	0.49
1:A:570:THR:HG22	1:A:623:ALA:HA	1.94	0.49
1:B:340:LEU:HG	1:B:646:MET:HG2	1.94	0.49
1:A:658:LYS:NZ	1:A:729:ASP:OD1	2.44	0.49
1:B:337:THR:CG2	1:B:646:MET:HE2	2.41	0.49
1:B:550:ASN:N	1:B:550:ASN:HD22	2.11	0.49
1:B:661:LEU:HG	1:B:728:VAL:HG21	1.94	0.49
1:B:667:LEU:HD13	1:B:721:GLU:HA	1.95	0.48
1:B:319:SER:C	1:B:321:PHE:N	2.70	0.48
1:A:736:LEU:CD1	1:B:736:LEU:HD12	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:MET:HG3	1:B:481:GLU:CB	2.44	0.48
1:B:581:TYR:O	1:B:585:VAL:HG23	2.13	0.48
1:B:378:VAL:HG23	1:B:425:VAL:HG23	1.96	0.48
1:B:508:ASN:HD21	1:B:549:ASP:H	1.62	0.48
1:A:627:ASN:HD22	1:A:629:VAL:H	1.62	0.48
1:A:424:VAL:HG12	1:A:455:GLN:NE2	2.29	0.47
1:A:680:TRP:CD2	1:A:687:PRO:HB3	2.49	0.47
1:B:404:MET:HB2	1:B:407:GLN:OE1	2.15	0.47
1:B:438:ASP:O	1:B:439:GLY:C	2.57	0.47
1:B:424:VAL:HG23	1:B:456:ASP:HB2	1.97	0.47
1:A:407:GLN:O	1:A:408:VAL:HG23	2.15	0.47
1:A:488:VAL:HG23	1:A:490:VAL:HG23	1.96	0.47
1:A:542:ILE:CD1	1:A:564:ARG:HG2	2.45	0.47
1:A:580:ASP:O	1:A:581:TYR:C	2.58	0.47
1:A:681:HIS:O	1:A:682:HIS:C	2.58	0.47
1:B:424:VAL:HG13	1:B:425:VAL:N	2.30	0.47
1:B:599:VAL:O	1:B:605:LEU:HA	2.15	0.46
1:A:527:ARG:HH21	1:A:546:ILE:HD11	1.79	0.46
1:A:713:PRO:HG3	1:A:719:TYR:HE1	1.79	0.46
1:B:389:ILE:HA	1:B:408:VAL:O	2.15	0.46
1:A:424:VAL:HG22	1:A:425:VAL:N	2.31	0.46
1:A:554:LEU:CD1	1:A:582:LEU:HD13	2.46	0.46
1:A:579:LYS:O	1:A:580:ASP:C	2.58	0.46
1:B:586:LEU:HD23	1:B:590:LEU:HD12	1.98	0.46
1:A:504:MET:HE3	1:A:547:VAL:HG21	1.98	0.46
1:B:504:MET:HE3	1:B:547:VAL:CG2	2.45	0.46
1:B:352:GLY:O	1:B:476:HIS:CD2	2.68	0.45
1:A:663:CYS:HA	1:A:724:LYS:HB2	1.98	0.45
1:B:377:ALA:HA	1:B:423:ALA:HB1	1.97	0.45
1:A:627:ASN:HD22	1:A:629:VAL:N	2.14	0.45
1:B:375:GLY:O	1:B:410:ARG:HD2	2.17	0.45
1:A:452:ARG:HB3	1:A:455:GLN:NE2	2.32	0.45
1:B:318:MET:O	1:B:319:SER:CB	2.64	0.45
1:B:608:THR:HB	1:B:623:ALA:HB3	1.99	0.44
1:B:593:GLN:NE2	1:B:611:THR:OG1	2.45	0.44
1:B:393:SER:HB3	1:B:411:VAL:HG23	1.99	0.44
1:B:425:VAL:O	1:B:426:GLN:CB	2.65	0.44
1:B:717:GLU:N	1:B:717:GLU:OE1	2.51	0.44
1:A:518:LEU:HB3	1:A:519:PRO:HD2	1.98	0.44
1:A:716:THR:HG22	1:A:717:GLU:N	2.31	0.44
1:B:426:GLN:O	1:B:428:GLU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:MET:HB3	1:B:544:LEU:HB2	1.99	0.44
1:A:680:TRP:CZ2	1:A:687:PRO:HG3	2.52	0.44
1:B:605:LEU:HB3	1:B:606:PRO:HD3	1.99	0.44
1:B:665:VAL:O	1:B:665:VAL:HG23	2.18	0.44
1:B:726:GLU:O	1:B:728:VAL:HG23	2.17	0.44
1:B:425:VAL:O	1:B:426:GLN:HB2	2.17	0.43
1:A:696:MET:O	1:A:697:SER:C	2.61	0.43
1:A:629:VAL:O	1:A:629:VAL:HG12	2.18	0.43
1:B:319:SER:C	1:B:321:PHE:H	2.26	0.43
1:B:319:SER:O	1:B:321:PHE:N	2.51	0.43
1:A:424:VAL:HG23	1:A:456:ASP:CG	2.43	0.43
1:B:564:ARG:HH11	1:B:564:ARG:CG	2.31	0.43
1:A:337:THR:HG23	1:A:646:MET:HE2	2.01	0.43
1:B:350:GLY:O	1:B:353:ARG:HB2	2.18	0.43
1:B:403:VAL:HB	1:B:420:GLY:HA3	1.99	0.43
1:B:568:ILE:HD12	1:B:568:ILE:N	2.33	0.43
1:B:672:GLU:HB2	1:B:712:LEU:HB2	2.00	0.43
1:B:735:ARG:HH11	1:B:735:ARG:CB	2.31	0.42
1:A:468:GLU:HG2	1:A:469:CYS:N	2.33	0.42
1:A:526:ASN:N	1:A:526:ASN:HD22	2.17	0.42
1:A:614:ILE:O	1:A:615:ASP:C	2.63	0.42
1:B:735:ARG:HH11	1:B:735:ARG:HG3	1.84	0.42
1:A:424:VAL:HA	1:A:456:ASP:HB2	2.01	0.42
1:A:558:LEU:HD13	1:A:590:LEU:CD1	2.48	0.42
1:A:709:LEU:HB2	1:A:731:MET:HB3	2.01	0.42
1:A:710:LEU:HD11	1:A:728:VAL:HG21	2.00	0.42
1:A:410:ARG:HH21	1:B:576:MET:HE2	1.85	0.42
1:A:661:LEU:HD21	1:A:710:LEU:HD21	2.02	0.42
1:A:318:MET:O	1:A:319:SER:CB	2.68	0.42
1:A:612:LEU:CD1	1:A:614:ILE:HD11	2.48	0.42
1:A:365:LEU:HD12	1:A:366:PRO:HA	2.01	0.42
1:B:668:ASP:O	1:B:669:PRO:C	2.58	0.41
1:A:367:PRO:HG2	1:A:368:PHE:CD2	2.55	0.41
1:A:578:GLU:C	1:A:580:ASP:N	2.77	0.41
1:A:605:LEU:C	1:A:605:LEU:CD1	2.92	0.41
1:B:366:PRO:HG3	1:B:458:ARG:HB3	2.02	0.41
1:B:646:MET:HE3	1:B:646:MET:HB2	1.93	0.41
1:A:605:LEU:HB3	1:A:606:PRO:HD3	2.03	0.41
1:A:620:ILE:HD11	1:A:646:MET:CE	2.48	0.41
1:A:662:SER:OG	1:A:690:GLN:NE2	2.54	0.41
1:B:567:VAL:HG22	1:B:620:ILE:CG1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:ASP:OD2	1:B:386:ASP:N	2.43	0.41
1:A:561:GLY:C	1:A:568:ILE:HD11	2.46	0.41
1:B:326:MET:O	1:B:327:ASP:C	2.64	0.41
1:B:430:THR:HA	1:B:446:ARG:O	2.21	0.41
1:B:530:LEU:O	1:B:534:ILE:HG23	2.20	0.41
1:A:376:TYR:HA	1:A:409:MET:O	2.21	0.41
1:A:355:LEU:CD2	1:A:493:VAL:HG11	2.51	0.40
1:A:421:ALA:C	1:A:422:ASP:OD1	2.64	0.40
1:A:432:LEU:HA	1:A:445:VAL:HA	2.03	0.40
1:A:531:LEU:CD2	1:A:541:THR:HB	2.51	0.40
1:A:736:LEU:HD11	1:B:736:LEU:HD12	2.03	0.40
1:B:384:PRO:O	1:B:385:GLY:O	2.39	0.40
1:B:435:GLU:HA	1:B:442:GLU:HA	2.03	0.40
1:B:374:ASP:OD1	1:B:427:VAL:HG23	2.21	0.40
1:B:390:ILE:HG23	1:B:407:GLN:HB3	2.04	0.40
1:B:718:GLN:HG3	1:B:719:TYR:N	2.37	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	399/419 (95%)	365 (92%)	23 (6%)	11 (3%)	4	9
1	B	417/419 (100%)	364 (87%)	36 (9%)	17 (4%)	2	5
All	All	816/838 (97%)	729 (89%)	59 (7%)	28 (3%)	3	7

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	SER
1	A	413	THR

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Mol	Chain	Res	Type
1	A	456	ASP
1	B	319	SER
1	B	385	GLY
1	B	424	VAL
1	B	425	VAL
1	B	443	LEU
1	A	422	ASP
1	A	574	VAL
1	A	577	GLY
1	A	696	MET
1	A	697	SER
1	B	426	GLN
1	B	719	TYR
1	B	428	GLU
1	B	439	GLY
1	B	448	LEU
1	B	682	HIS
1	B	696	MET
1	B	698	SER
1	A	424	VAL
1	A	453	PRO
1	B	320	PRO
1	B	384	PRO
1	B	451	ALA
1	A	572	GLY
1	B	427	VAL

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	334/356 (94%)	309 (92%)	25 (8%)	12	31
1	B	338/356 (95%)	312 (92%)	26 (8%)	12	30
All	All	672/712 (94%)	621 (92%)	51 (8%)	12	30

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	318	MET
1	A	326	MET
1	A	334	LEU
1	A	408	VAL
1	A	424	VAL
1	A	465	LYS
1	A	466	ARG
1	A	484	LEU
1	A	498	PHE
1	A	500	VAL
1	A	534	ILE
1	A	549	ASP
1	A	552	ASP
1	A	554	LEU
1	A	579	LYS
1	A	599	VAL
1	A	605	LEU
1	A	612	LEU
1	A	627	ASN
1	A	647	GLN
1	A	660	ARG
1	A	667	LEU
1	A	717	GLU
1	A	718	GLN
1	A	722	LEU
1	B	353	ARG
1	B	386	ASP
1	B	408	VAL
1	B	458	ARG
1	B	477	MET
1	B	484	LEU
1	B	493	VAL
1	B	500	VAL
1	B	534	ILE
1	B	550	ASN
1	B	560	GLU
1	B	564	ARG
1	B	574	VAL
1	B	576	MET
1	B	578	GLU
1	B	599	VAL
1	B	614	ILE
1	B	632	VAL

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Mol	Chain	Res	Type
1	B	667	LEU
1	B	679	THR
1	B	694	ASN
1	B	717	GLU
1	B	718	GLN
1	B	720	VAL
1	B	722	LEU
1	B	735	ARG

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

Mol	Chain	Res	Type
1	A	455	GLN
1	A	508	ASN
1	A	526	ASN
1	A	556	ASN
1	A	591	HIS
1	A	627	ASN
1	A	690	GLN
1	B	476	HIS
1	B	508	ASN
1	B	526	ASN
1	B	550	ASN
1	B	556	ASN
1	B	591	HIS
1	B	593	GLN
1	B	627	ASN
1	B	636	ASN
1	B	707	ASN
1	B	723	HIS

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 [i](#)

There are no oligosaccharides 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

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	A	405/419 (96%)	0.46	24 (5%) 28 25	49, 64, 71, 79	0
1	B	419/419 (100%)	0.66	39 (9%) 14 12	55, 65, 71, 74	0
All	All	824/838 (98%)	0.56	63 (7%) 20 17	49, 65, 71, 79	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	696	MET	4.7
1	B	695	GLN	4.6
1	A	697	SER	4.5
1	B	686	LEU	4.0
1	B	378	VAL	3.9
1	A	695	GLN	3.6
1	A	574	VAL	3.6
1	A	573	GLY	3.6
1	B	447	ILE	3.2
1	B	576	MET	3.1
1	B	438	ASP	3.0
1	B	318	MET	3.0
1	A	736	LEU	2.9
1	B	549	ASP	2.9
1	A	425	VAL	2.9
1	A	686	LEU	2.9
1	A	687	PRO	2.8
1	B	687	PRO	2.8
1	B	381	ALA	2.8
1	B	578	GLU	2.8
1	B	577	GLY	2.7
1	B	422	ASP	2.7
1	A	577	GLY	2.7
1	B	445	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	685	PRO	2.7
1	A	383	GLY	2.7
1	A	575	SER	2.7
1	B	408	VAL	2.7
1	B	683	GLN	2.6
1	A	436	SER	2.6
1	B	421	ALA	2.6
1	A	685	PRO	2.6
1	A	566	ASP	2.5
1	A	433	ILE	2.5
1	B	699	ARG	2.5
1	A	576	MET	2.4
1	B	539	TYR	2.4
1	B	581	TYR	2.4
1	A	432	LEU	2.3
1	A	696	MET	2.3
1	A	700	LEU	2.3
1	B	682	HIS	2.3
1	B	440	THR	2.3
1	B	540	PRO	2.3
1	B	663	CYS	2.3
1	B	320	PRO	2.3
1	B	694	ASN	2.2
1	B	388	PHE	2.2
1	A	402	THR	2.2
1	B	707	ASN	2.2
1	B	684	GLU	2.1
1	B	319	SER	2.1
1	B	354	VAL	2.1
1	B	419	CYS	2.1
1	A	548	GLY	2.1
1	B	377	ALA	2.1
1	B	423	ALA	2.1
1	A	690	GLN	2.1
1	B	568	ILE	2.1
1	A	567	VAL	2.1
1	B	573	GLY	2.0
1	A	564	ARG	2.0
1	B	566	ASP	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.