Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:24 am BST

PDB ID	:	2FU3
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 following versions of software and data (see references ⓘ) were used in the production of this report:

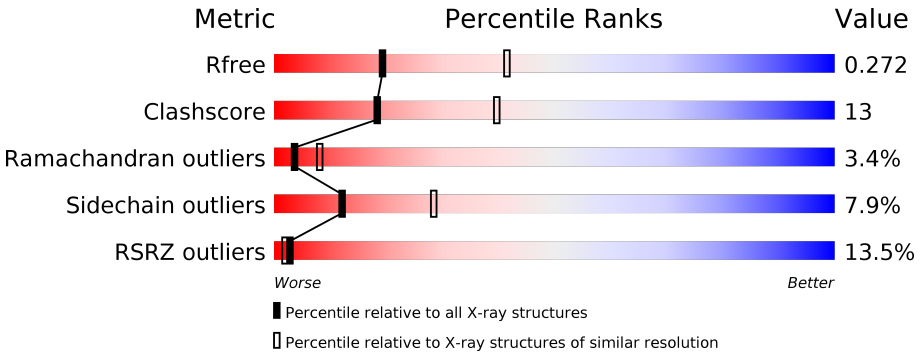
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 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 <=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	13% 69% 24%
1	B	419	14% 68% 25% 6%

2 Entry composition (i)

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.

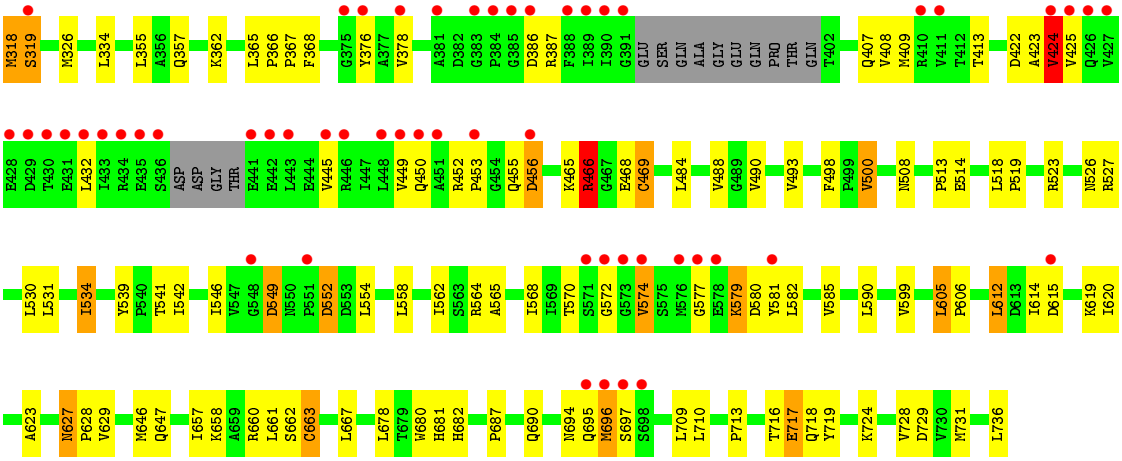
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	37	Total	O	0	0
			37	37		
2	B	29	Total	O	0	0
			29	29		

3 Residue-property plots (i)

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.

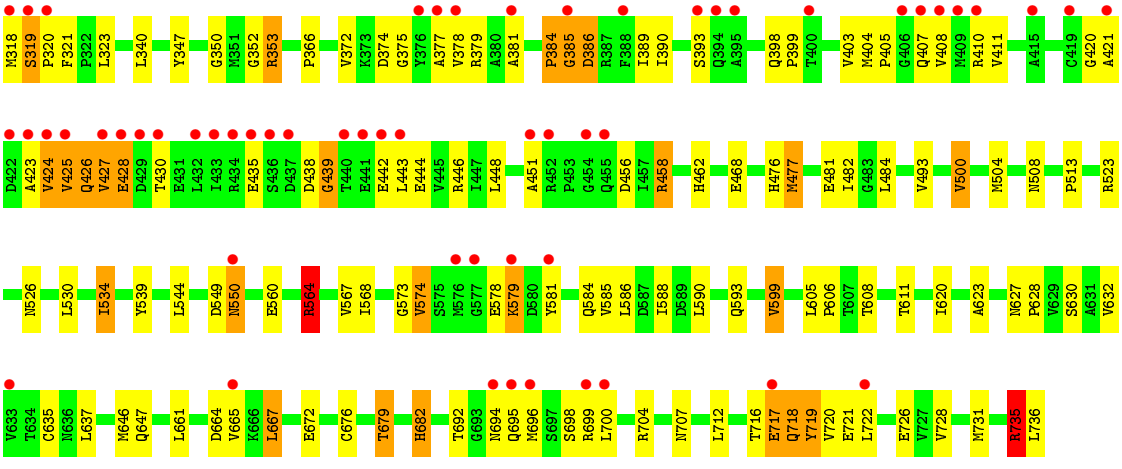
- Molecule 1: gephyrin

Chain A:



- Molecule 1: gephyrin

Chain B:



4 Data and refinement statistics (i)

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 39.92 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.70) 96.9 (39.92-2.38)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.202 , 0.273 0.209 , 0.272	Depositor DCC
R_{free} test set	1748 reflections (4.99%)	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 , 71.0	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	0.94	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.*

[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

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	1.03	4/3112 (0.1%)	0.76	1/4233 (0.0%)
1	B	1.03	6/3198 (0.2%)	0.81	2/4355 (0.0%)
All	All	1.03	10/6310 (0.2%)	0.78	3/8588 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	676	CYS	CB-SG	-6.58	1.71	1.82
1	B	635	CYS	CB-SG	-6.56	1.71	1.82
1	A	514	GLU	CB-CG	6.28	1.64	1.52
1	A	469	CYS	CB-SG	-6.01	1.72	1.82
1	B	647	GLN	CB-CG	-5.53	1.37	1.52
1	A	663	CYS	CB-SG	-5.52	1.72	1.81
1	A	424	VAL	CA-CB	5.34	1.66	1.54
1	B	500	VAL	CB-CG1	-5.28	1.41	1.52
1	B	574	VAL	CA-CB	5.09	1.65	1.54
1	B	468	GLU	CG-CD	5.07	1.59	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	735	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	A	466	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	B	564	ARG	NE-CZ-NH1	5.03	122.81	120.30

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	79	0
1	B	3137	0	3127	91	0
2	A	37	0	0	1	0
2	B	29	0	0	1	0
All	All	6257	0	6199	165	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 (165) 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: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: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:424:VAL:CG2	1:B:456:ASP:HB2	2.22	0.69
1:B:423:ALA:O	1:B:424:VAL:HB	1.92	0.68
1:B:718:GLN:O	1:B:719:TYR:C	2.33	0.67
1:B:378:VAL:O	1:B:423:ALA:HA	1.95	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: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:A:562:ILE:O	1:A:619:LYS:NZ	2.31	0.62
1:A:466:ARG:HG3	1:A:466:ARG:HH21	1.66	0.61
1:A:423:ALA:N	2:A:34:HOH:O	2.32	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:A:526:ASN:O	1:A:527:ARG:C	2.41	0.58
1:B:513:PRO:HA	1:B:523:ARG:HD3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:ILE:HD12	1:B:442:GLU:O	2.04	0.58
1:B:564:ARG:HH11	1:B:564:ARG:HG2	1.68	0.57
1:A:552:ASP:N	1:A:552:ASP:OD2	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:HH11	1:B:735:ARG:HB2	1.70	0.56
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:696:MET:CE	1:B:462:HIS:CE1	2.89	0.55
1:A:574:VAL:HA	1:A:579:LYS:HB2	1.87	0.54
1:A:680:TRP:CE2	1:A:687:PRO:HB3	2.42	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: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:CG	1:B:735:ARG:HH11	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:605:LEU:C	1:A:605:LEU:HD13	2.32	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:LYS:NZ	1:A:729:ASP:OD1	2.44	0.49
1:B:550:ASN:HD22	1:B:550:ASN:N	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:477:MET:HG3	1:B:481:GLU:CB	2.44	0.48
1:A:736:LEU:CD1	1:B:736:LEU:HD12	2.43	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: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:B:424:VAL:HG13	1:B:425:VAL:N	2.30	0.47
1:B:379:ARG:C	1:B:381:ALA:H	2.17	0.46
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:B:586:LEU:HD23	1:B:590:LEU:HD12	1.98	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:A:386:ASP:C	1:A:387:ARG:HG3	2.37	0.45
1:A:696:MET:HE1	1:B:462:HIS:CE1	2.52	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:OE1	1:B:717:GLU:N	2.51	0.44
1:A:518:LEU:HB3	1:A:519:PRO:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:504:MET:HB3	1:B:544:LEU:HB2	1.99	0.44
1:A:620:ILE:HD11	1:A:646:MET:CE	2.48	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:629:VAL:HG12	1:A:629:VAL:O	2.18	0.43
1:B:319:SER:O	1:B:321:PHE:N	2.51	0.43
1:B:319:SER:C	1:B:321:PHE:N	2.70	0.43
1:B:564:ARG:HH11	1:B:564:ARG:CG	2.31	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:N	1:B:568:ILE:HD12	2.33	0.43
1:B:672:GLU:HB2	1:B:712:LEU:HB2	2.00	0.43
1:B:438:ASP:O	1:B:439:GLY:C	2.57	0.42
1:A:646:MET:HB2	1:A:646:MET:HE3	1.93	0.42
1:B:735:ARG:CB	1:B:735:ARG:HH11	2.31	0.42
1:A:468:GLU:HG2	1:A:469:CYS:N	2.33	0.42
1:A:526:ASN:HD22	1:A:526:ASN:N	2.17	0.42
1:B:735:ARG:HG3	1:B:735:ARG:HH11	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:B:620:ILE:CD1	1:B:646:MET:HE1	2.49	0.42
1:A:710:LEU:HD11	1:A:728:VAL:HG21	2.00	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:580:ASP:O	1:A:581:TYR:C	2.58	0.42
1:A:612:LEU:CD1	1:A:614:ILE:HD11	2.48	0.42
1:A:681:HIS:O	1:A:682:HIS:C	2.58	0.42
1:A:696:MET:HE3	1:B:462:HIS:CE1	2.55	0.42
1:A:365:LEU:HD12	1:A:366:PRO:HA	2.01	0.42
1:A:620:ILE:CD1	1:A:646:MET:HE2	2.50	0.42
1:A:367:PRO:HG2	1:A:368:PHE:CD2	2.55	0.41
1:B:366:PRO:HG3	1:B:458:ARG:HB3	2.02	0.41
1:A:605:LEU:HB3	1:A:606:PRO:HD3	2.03	0.41
1:A:579:LYS:O	1:A:580:ASP:C	2.58	0.41
1:A:662:SER:OG	1:A:690:GLN:NE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:VAL:HG22	1:B:620:ILE:CG1	2.50	0.41
1:B:386:ASP:N	1:B:386:ASP:OD2	2.43	0.41
1:B:530:LEU:O	1:B:534:ILE:HG23	2.20	0.41
1:B:430:THR:HA	1:B:446:ARG:O	2.21	0.41
1:B:637:LEU:HD23	1:B:731:MET:CE	2.50	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: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:390:ILE:HG23	1:B:407:GLN:HB3	2.04	0.40
1:B:374:ASP:OD1	1:B:427:VAL:HG23	2.21	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%)	5 11
1	B	417/419 (100%)	364 (87%)	36 (9%)	17 (4%)	3 6
All	All	816/838 (97%)	729 (89%)	59 (7%)	28 (3%)	3 8

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	SER
1	A	413	THR
1	A	456	ASP

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Mol	Chain	Res	Type
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 (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	334/356 (94%)	310 (93%)	24 (7%)	14	34
1	B	338/356 (95%)	309 (91%)	29 (9%)	10	24
All	All	672/712 (94%)	619 (92%)	53 (8%)	12	28

All (53) 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	357	GLN
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	579	LYS
1	A	599	VAL
1	A	605	LEU
1	A	612	LEU
1	A	615	ASP
1	A	627	ASN
1	A	647	GLN
1	A	660	ARG
1	A	667	LEU
1	A	694	ASN
1	A	717	GLU
1	A	718	GLN
1	B	353	ARG
1	B	386	ASP
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	578	GLU
1	B	579	LYS
1	B	599	VAL
1	B	632	VAL
1	B	664	ASP
1	B	667	LEU
1	B	679	THR

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Mol	Chain	Res	Type
1	B	682	HIS
1	B	694	ASN
1	B	695	GLN
1	B	699	ARG
1	B	707	ASN
1	B	717	GLU
1	B	718	GLN
1	B	720	VAL
1	B	722	LEU
1	B	735	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) 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	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	627	ASN
1	B	707	ASN
1	B	723	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 carbohydrates 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, 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	A	405/419 (96%)	0.66	54 (13%)	3 2	49, 64, 71, 79	0
1	B	419/419 (100%)	0.65	57 (13%)	3 2	55, 65, 71, 74	0
All	All	824/838 (98%)	0.65	111 (13%)	3 2	49, 65, 71, 79	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	428	GLU	11.2
1	B	695	GLN	9.8
1	B	381	ALA	8.7
1	A	383	GLY	8.7
1	A	433	ILE	8.0
1	A	697	SER	7.8
1	A	425	VAL	7.7
1	A	386	ASP	7.7
1	B	696	MET	7.7
1	A	695	GLN	7.5
1	B	432	LEU	6.7
1	A	424	VAL	6.3
1	B	400	THR	5.8
1	A	431	GLU	5.7
1	B	318	MET	5.4
1	B	430	THR	5.2
1	B	408	VAL	5.2
1	A	443	LEU	5.2
1	A	576	MET	5.1
1	A	441	GLU	5.1
1	B	376	TYR	5.1
1	B	423	ALA	5.0
1	A	390	ILE	5.0
1	B	378	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	425	VAL	4.7
1	A	427	VAL	4.7
1	A	442	GLU	4.6
1	B	694	ASN	4.6
1	A	436	SER	4.6
1	B	576	MET	4.5
1	B	419	CYS	4.5
1	A	698	SER	4.4
1	A	448	LEU	4.3
1	B	717	GLU	4.2
1	B	319	SER	4.2
1	B	577	GLY	4.2
1	B	385	GLY	4.2
1	A	426	GLN	4.1
1	B	581	TYR	4.0
1	B	415	ALA	4.0
1	B	437	ASP	4.0
1	B	455	GLN	3.9
1	A	376	TYR	3.9
1	A	450	GLN	3.9
1	B	434	ARG	3.8
1	A	319	SER	3.8
1	A	451	ALA	3.8
1	A	577	GLY	3.8
1	B	377	ALA	3.8
1	A	548	GLY	3.7
1	B	451	ALA	3.7
1	A	389	ILE	3.7
1	A	435	GLU	3.6
1	A	573	GLY	3.6
1	A	432	LEU	3.5
1	A	578	GLU	3.5
1	A	574	VAL	3.5
1	A	430	THR	3.4
1	B	422	ASP	3.4
1	A	378	VAL	3.3
1	A	375	GLY	3.2
1	B	320	PRO	3.2
1	B	429	ASP	3.2
1	B	388	PHE	3.1
1	B	395	ALA	3.1
1	B	433	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	388	PHE	3.0
1	B	443	LEU	3.0
1	B	435	GLU	2.9
1	B	441	GLU	2.9
1	A	571	SER	2.9
1	A	572	GLY	2.9
1	A	385	GLY	2.8
1	B	406	GLY	2.8
1	A	384	PRO	2.8
1	B	427	VAL	2.7
1	B	550	ASN	2.7
1	A	410	ARG	2.7
1	B	421	ALA	2.7
1	A	391	GLY	2.6
1	A	696	MET	2.6
1	B	665	VAL	2.6
1	B	700	LEU	2.6
1	B	428	GLU	2.6
1	B	579	LYS	2.6
1	A	551	PRO	2.6
1	B	452	ARG	2.5
1	A	445	VAL	2.5
1	B	410	ARG	2.5
1	B	407	GLN	2.5
1	B	440	THR	2.5
1	A	615	ASP	2.4
1	B	409	MET	2.4
1	B	454	GLY	2.4
1	A	434	ARG	2.4
1	B	633	VAL	2.4
1	A	446	ARG	2.3
1	A	456	ASP	2.3
1	B	699	ARG	2.3
1	A	581	TYR	2.2
1	B	393	SER	2.2
1	A	449	VAL	2.2
1	B	424	VAL	2.2
1	B	722	LEU	2.2
1	B	442	GLU	2.2
1	A	381	ALA	2.2
1	A	453	PRO	2.1
1	B	394	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	411	VAL	2.1
1	A	429	ASP	2.0
1	B	436	SER	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.