W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:07 AM GMT

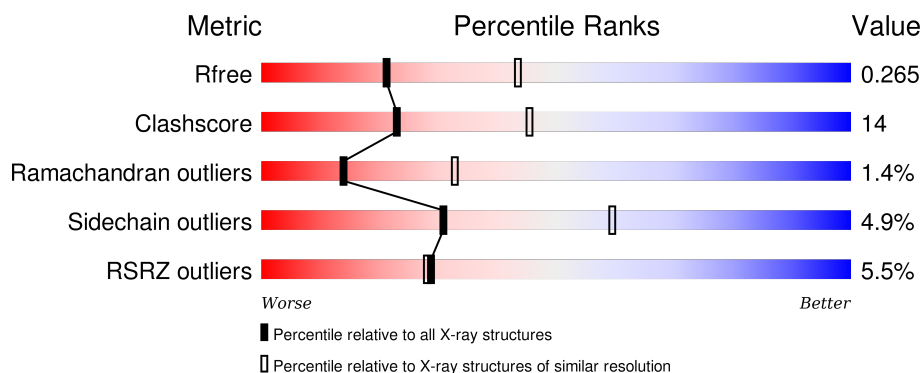|		
PDB ID	:	3KY9
Title	:	Autoinhibited Vav1
Authors	:	Tomchick, D.R.; Rosen, M.K.; Machius, M.; Yu, B.
Deposited on	:	2009-12-04
Resolution	:	2.73 Å(reported)

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 2.73 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	Percentile Ranks	Value
Rfree		0.265
Clashscore		14
Ramachandran outliers		1.4%
Sidechain outliers		4.9%
RSRZ outliers		5.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3050 (2.78-2.70)
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

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. 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	587	5% / 61% / 26% / · / 10%
1	B	587	5% / 61% / 27% / · / 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8813 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 Proto-oncogene vav.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	530	Total	C	N	O	S	0	0	0
			4368	2757	769	805	37			
1	B	541	Total	C	N	O	S	0	0	0
			4441	2797	781	826	37			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P15498
A	-1	HIS	-	EXPRESSION TAG	UNP P15498
A	0	MET	-	EXPRESSION TAG	UNP P15498
A	1	LYS	-	EXPRESSION TAG	UNP P15498
A	26	GLU	ASP	CONFLICT	UNP P15498
B	-3	GLY	-	EXPRESSION TAG	UNP P15498
B	-2	HIS	-	EXPRESSION TAG	UNP P15498
B	-1	MET	-	EXPRESSION TAG	UNP P15498
B	0	LYS	-	EXPRESSION TAG	UNP P15498
B	26	GLU	ASP	CONFLICT	UNP P15498

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

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 errors 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: Proto-oncogene vav
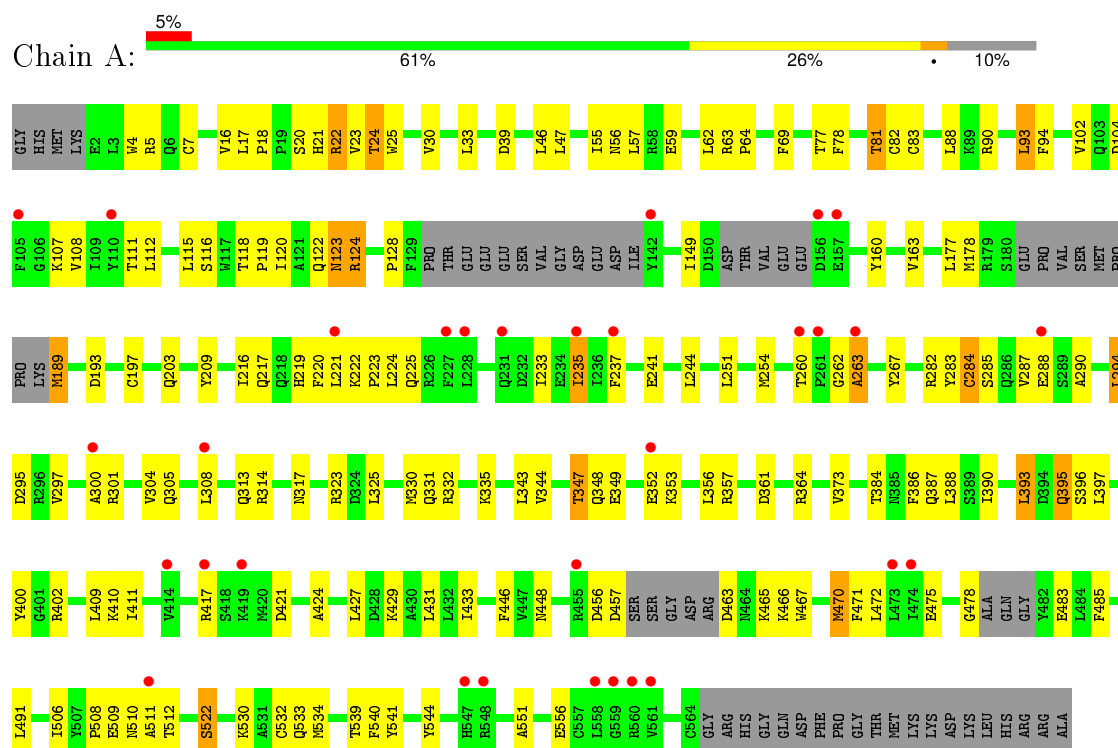
- Molecule 1: Proto-oncogene vav
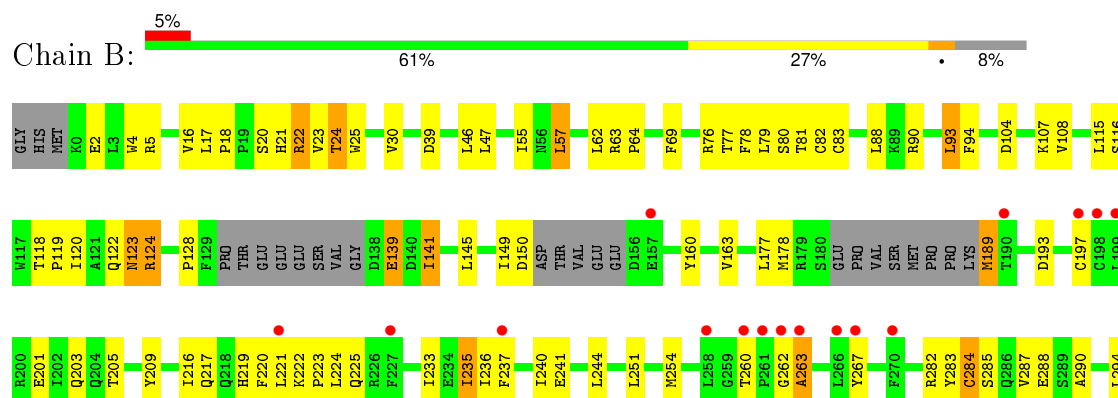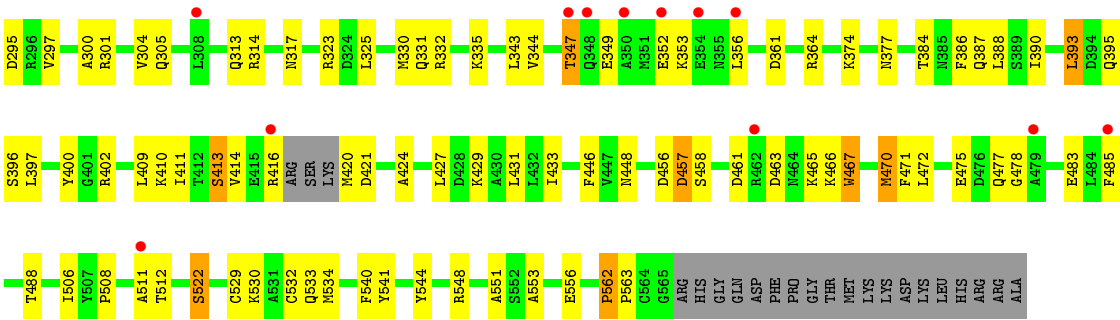
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.38Å 58.74Å 160.72Å 90.00° 97.31° 90.00°	Depositor
Resolution (Å)	47.29 – 2.73 47.29 – 2.73	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.29-2.73) 97.6 (47.29-2.73)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.59 (at 2.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.223 , 0.271 0.217 , 0.265	Depositor DCC
R_{free} test set	1681 reflections (4.05%)	DCC
Wilson B-factor (Å^2)	72.6	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 63.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.50, <L^2> = 0.33$	Xtriage
Outliers	0 of 41525 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8813	wwPDB-VP
Average B, all atoms (Å^2)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.71% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.42	1/4448 (0.0%)	0.57	0/5979
1	B	0.42	1/4522 (0.0%)	0.57	0/6080
All	All	0.42	2/8970 (0.0%)	0.57	0/12059

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	284	CYS	CB-SG	6.37	1.93	1.82
1	B	284	CYS	CB-SG	5.54	1.91	1.82

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	4368	0	4313	119	0
1	B	4441	0	4372	125	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
All	All	8813	0	8685	237	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 14.

All (237) 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:189:MET:HG3	1:B:193:ASP:HB2	1.46	0.98
1:A:189:MET:HG3	1:A:193:ASP:HB2	1.48	0.93
1:B:78:PHE:O	1:B:82:CYS:HB2	1.75	0.85
1:B:150:ASP:HB3	1:B:488:THR:HG21	1.57	0.84
1:A:78:PHE:O	1:A:82:CYS:HB2	1.79	0.82
1:A:522:SER:HB3	1:A:541:TYR:H	1.45	0.81
1:B:522:SER:HB3	1:B:541:TYR:H	1.45	0.80
1:B:62:LEU:O	1:B:63:ARG:HD3	1.83	0.79
1:A:62:LEU:O	1:A:63:ARG:HD3	1.85	0.77
1:A:393:LEU:HD11	1:A:397:LEU:HD21	1.66	0.76
1:B:458:SER:HB2	1:B:461:ASP:HB3	1.69	0.75
1:B:393:LEU:HD11	1:B:397:LEU:HD21	1.67	0.75
1:B:352:GLU:OE1	1:B:352:GLU:HA	1.90	0.71
1:B:221:LEU:HD22	1:B:233:ILE:HD11	1.73	0.70
1:B:21:HIS:O	1:B:24:THR:HB	1.92	0.70
1:B:458:SER:CB	1:B:461:ASP:HB3	2.22	0.70
1:A:119:PRO:O	1:A:123:ASN:HB2	1.93	0.69
1:B:118:THR:HG22	1:B:120:ILE:H	1.58	0.69
1:A:284:CYS:SG	1:A:330:MET:HG2	2.33	0.69
1:A:102:VAL:HG11	1:A:149:ILE:HD11	1.74	0.68
1:A:221:LEU:HD22	1:A:233:ILE:HD11	1.75	0.68
1:A:102:VAL:HG11	1:A:149:ILE:CD1	2.24	0.68
1:A:21:HIS:O	1:A:24:THR:HB	1.92	0.68
1:A:118:THR:HG22	1:A:120:ILE:H	1.59	0.67
1:B:284:CYS:SG	1:B:330:MET:HG2	2.34	0.67
1:A:77:THR:O	1:A:81:THR:HG23	1.94	0.67
1:A:411:ILE:HD11	1:A:433:ILE:HD12	1.77	0.67
1:A:352:GLU:OE1	1:A:352:GLU:HA	1.93	0.67
1:B:119:PRO:O	1:B:123:ASN:HB2	1.94	0.67
1:A:284:CYS:SG	1:A:330:MET:HA	2.34	0.67
1:A:203:GLN:HA	1:A:254:MET:HE1	1.78	0.66
1:B:216:ILE:HD11	1:B:325:LEU:HB3	1.77	0.66
1:A:221:LEU:HD13	1:A:237:PHE:HA	1.79	0.65
1:B:2:GLU:H	1:B:2:GLU:CD	1.98	0.65
1:B:411:ILE:HD11	1:B:433:ILE:HD12	1.77	0.65
1:B:284:CYS:SG	1:B:330:MET:HA	2.36	0.65
1:A:347:THR:O	1:A:353:LYS:HE2	1.96	0.65
1:A:216:ILE:HD11	1:A:325:LEU:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:VAL:HG13	1:B:288:GLU:N	2.12	0.64
1:B:77:THR:O	1:B:81:THR:HG23	1.99	0.63
1:B:221:LEU:HD13	1:B:237:PHE:HA	1.79	0.63
1:A:287:VAL:HG13	1:A:288:GLU:N	2.14	0.63
1:A:357:ARG:HB3	1:B:548:ARG:NH1	2.14	0.63
1:A:384:THR:O	1:A:388:LEU:HG	1.99	0.62
1:B:347:THR:O	1:B:353:LYS:HE2	2.00	0.61
1:A:216:ILE:HA	1:A:220:PHE:HD2	1.66	0.60
1:B:203:GLN:HA	1:B:254:MET:HE1	1.83	0.60
1:B:472:LEU:HD23	1:B:483:GLU:HB3	1.82	0.60
1:A:472:LEU:HD23	1:A:483:GLU:HB3	1.82	0.60
1:A:216:ILE:O	1:A:220:PHE:HB2	2.02	0.60
1:B:287:VAL:HG13	1:B:288:GLU:H	1.66	0.59
1:A:508:PRO:HG2	1:A:544:TYR:CE2	2.37	0.59
1:B:216:ILE:O	1:B:220:PHE:HB2	2.02	0.59
1:B:4:TRP:NE1	1:B:30:VAL:HG22	2.17	0.58
1:A:251:LEU:HD12	1:A:254:MET:HE2	1.85	0.58
1:A:313:GLN:O	1:A:317:ASN:HA	2.04	0.58
1:B:39:ASP:OD1	1:B:39:ASP:O	2.22	0.58
1:A:122:GLN:C	1:A:124:ARG:H	2.07	0.58
1:A:411:ILE:CD1	1:A:433:ILE:HD12	2.33	0.58
1:A:357:ARG:HB3	1:B:548:ARG:NH2	2.19	0.57
1:B:122:GLN:C	1:B:124:ARG:H	2.08	0.57
1:A:427:LEU:N	1:A:427:LEU:HD12	2.20	0.57
1:A:235:ILE:CG2	1:A:290:ALA:HB2	2.35	0.57
1:B:530:LYS:HE3	1:B:551:ALA:HA	1.86	0.57
1:B:94:PHE:HB3	1:B:107:LYS:HG3	1.87	0.57
1:A:348:GLN:NE2	1:B:477:GLN:OE1	2.37	0.57
1:B:386:PHE:O	1:B:390:ILE:HG13	2.05	0.56
1:A:386:PHE:O	1:A:390:ILE:HG13	2.05	0.56
1:A:530:LYS:HE3	1:A:551:ALA:HA	1.87	0.56
1:B:283:TYR:C	1:B:285:SER:H	2.09	0.56
1:A:287:VAL:HG13	1:A:288:GLU:H	1.68	0.56
1:A:357:ARG:HB3	1:B:548:ARG:CZ	2.35	0.56
1:B:244:LEU:HD12	1:B:244:LEU:O	2.05	0.56
1:A:475:GLU:OE1	1:A:478:GLY:HA3	2.04	0.56
1:A:508:PRO:CG	1:A:544:TYR:CE2	2.89	0.56
1:B:384:THR:O	1:B:388:LEU:HG	2.06	0.56
1:A:508:PRO:HD2	1:A:511:ALA:HB2	1.87	0.56
1:B:313:GLN:O	1:B:317:ASN:HA	2.06	0.56
1:B:411:ILE:CD1	1:B:433:ILE:HD12	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:TYR:C	1:A:285:SER:H	2.10	0.55
1:B:466:LYS:O	1:B:467:TRP:HB2	2.06	0.55
1:A:39:ASP:OD1	1:A:39:ASP:O	2.24	0.54
1:B:149:ILE:HG22	1:B:150:ASP:N	2.21	0.54
1:A:387:GLN:OE1	1:A:396:SER:HA	2.08	0.54
1:A:244:LEU:HD12	1:A:244:LEU:O	2.08	0.54
1:B:216:ILE:HA	1:B:220:PHE:HD2	1.72	0.54
1:B:235:ILE:CG2	1:B:290:ALA:HB2	2.38	0.54
1:B:203:GLN:HA	1:B:254:MET:CE	2.39	0.53
1:A:94:PHE:HB3	1:A:107:LYS:HG3	1.90	0.53
1:B:304:VAL:HG12	1:B:305:GLN:N	2.23	0.53
1:B:251:LEU:HD12	1:B:254:MET:HE2	1.90	0.53
1:B:475:GLU:OE1	1:B:478:GLY:HA3	2.09	0.52
1:A:373:VAL:HG22	1:A:539:THR:HG23	1.91	0.52
1:B:387:GLN:OE1	1:B:396:SER:HA	2.10	0.52
1:A:402:ARG:NH2	1:A:540:PHE:O	2.43	0.52
1:A:470:MET:HE3	1:A:471:PHE:HA	1.91	0.52
1:A:357:ARG:HB3	1:B:548:ARG:HH12	1.75	0.52
1:B:343:LEU:O	1:B:347:THR:OG1	2.28	0.52
1:B:118:THR:HG22	1:B:120:ILE:N	2.24	0.52
1:B:297:VAL:HG12	1:B:297:VAL:O	2.10	0.51
1:B:508:PRO:HD2	1:B:511:ALA:HB2	1.91	0.51
1:A:466:LYS:O	1:A:467:TRP:HB2	2.10	0.51
1:B:201:GLU:O	1:B:205:THR:HG23	2.10	0.51
1:A:235:ILE:HG21	1:A:290:ALA:HB2	1.93	0.51
1:A:94:PHE:CD2	1:A:108:VAL:HA	2.44	0.51
1:B:150:ASP:CB	1:B:488:THR:HG21	2.37	0.51
1:B:349:GLU:OE1	1:B:352:GLU:HG2	2.10	0.51
1:A:300:ALA:O	1:A:301:ARG:HG3	2.11	0.51
1:B:39:ASP:HB2	1:B:64:PRO:HG2	1.93	0.51
1:B:94:PHE:CD2	1:B:108:VAL:HA	2.46	0.50
1:B:427:LEU:N	1:B:427:LEU:HD12	2.26	0.50
1:A:297:VAL:HG12	1:A:297:VAL:O	2.12	0.50
1:B:352:GLU:OE1	1:B:352:GLU:CA	2.59	0.50
1:A:39:ASP:HB2	1:A:64:PRO:HG2	1.93	0.50
1:A:262:GLY:O	1:A:263:ALA:HB3	2.12	0.50
1:A:116:SER:HB2	1:A:128:PRO:HA	1.93	0.50
1:B:262:GLY:O	1:B:263:ALA:HB3	2.12	0.50
1:A:16:VAL:HG21	1:A:46:LEU:HB2	1.94	0.49
1:A:304:VAL:HG12	1:A:305:GLN:N	2.27	0.49
1:A:118:THR:HG22	1:A:120:ILE:N	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:VAL:HG13	1:B:288:GLU:HG3	1.94	0.49
1:A:203:GLN:HA	1:A:254:MET:CE	2.42	0.49
1:A:209:TYR:CD2	1:A:332:ARG:HG2	2.48	0.48
1:B:300:ALA:O	1:B:301:ARG:HG3	2.12	0.48
1:A:556:GLU:H	1:A:556:GLU:CD	2.16	0.48
1:A:352:GLU:OE1	1:A:352:GLU:CA	2.61	0.48
1:A:7:CYS:SG	1:A:112:LEU:HD12	2.54	0.48
1:A:400:TYR:CE2	1:A:446:PHE:HZ	2.32	0.48
1:B:400:TYR:CE2	1:B:446:PHE:HZ	2.31	0.48
1:A:4:TRP:NE1	1:A:30:VAL:HG22	2.29	0.48
1:B:470:MET:HE3	1:B:471:PHE:HA	1.95	0.48
1:B:402:ARG:NH2	1:B:540:PHE:O	2.46	0.47
1:A:90:ARG:HA	1:A:93:LEU:HD11	1.96	0.47
1:B:267:TYR:HB3	1:B:356:LEU:HD23	1.96	0.47
1:A:17:LEU:HD21	1:A:23:VAL:HG21	1.95	0.47
1:B:4:TRP:CE2	1:B:30:VAL:HG22	2.50	0.47
1:B:470:MET:HB3	1:B:485:PHE:CD1	2.50	0.47
1:A:160:TYR:O	1:A:163:VAL:HG22	2.14	0.47
1:A:219:HIS:HA	1:A:314:ARG:HH21	1.80	0.47
1:A:287:VAL:HG13	1:A:288:GLU:HG3	1.96	0.47
1:B:47:LEU:HD21	1:B:115:LEU:HD21	1.97	0.47
1:A:55:ILE:HG12	1:A:81:THR:HG21	1.97	0.47
1:A:349:GLU:OE1	1:A:352:GLU:HG2	2.15	0.47
1:A:209:TYR:CG	1:A:332:ARG:HG2	2.50	0.47
1:B:145:LEU:HA	1:B:145:LEU:HD23	1.72	0.47
1:A:357:ARG:CB	1:B:548:ARG:NH2	2.78	0.47
1:B:219:HIS:HA	1:B:314:ARG:HH21	1.79	0.47
1:B:22:ARG:HA	1:B:25:TRP:CD2	2.51	0.46
1:A:470:MET:HB3	1:A:485:PHE:CD1	2.50	0.46
1:A:343:LEU:O	1:A:347:THR:OG1	2.32	0.46
1:B:235:ILE:HG21	1:B:290:ALA:HB2	1.96	0.46
1:A:237:PHE:CZ	1:A:241:GLU:HG3	2.50	0.46
1:B:69:PHE:CD2	1:B:386:PHE:HE1	2.34	0.46
1:B:331:GLN:O	1:B:335:LYS:HG2	2.15	0.46
1:A:424:ALA:HB1	1:A:431:LEU:HD11	1.98	0.46
1:B:90:ARG:HA	1:B:93:LEU:HD11	1.97	0.46
1:B:529:CYS:SG	1:B:553:ALA:HA	2.56	0.46
1:B:457:ASP:HB3	1:B:470:MET:HE1	1.97	0.46
1:A:417:ARG:HD3	1:A:417:ARG:HA	1.56	0.46
1:B:216:ILE:HA	1:B:220:PHE:CD2	2.51	0.46
1:A:361:ASP:OD1	1:A:364:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ILE:HA	1:A:220:PHE:CD2	2.49	0.45
1:B:424:ALA:HB1	1:B:431:LEU:HD11	1.98	0.45
1:A:23:VAL:HG11	1:A:33:LEU:HA	1.99	0.45
1:A:16:VAL:CG2	1:A:46:LEU:HA	2.47	0.45
1:A:4:TRP:CH2	1:A:5:ARG:HD2	2.52	0.45
1:B:544:TYR:N	1:B:544:TYR:CD1	2.85	0.45
1:A:393:LEU:HD11	1:A:397:LEU:CD2	2.42	0.45
1:B:209:TYR:CD2	1:B:332:ARG:HG2	2.52	0.45
1:B:508:PRO:CG	1:B:544:TYR:CE2	3.00	0.44
1:A:463:ASP:OD2	1:A:465:LYS:HG3	2.17	0.44
1:B:30:VAL:HG21	1:B:141:ILE:HG21	1.99	0.44
1:B:556:GLU:H	1:B:556:GLU:CD	2.20	0.44
1:A:222:LYS:HB2	1:A:223:PRO:HD3	2.00	0.44
1:B:361:ASP:OD1	1:B:364:ARG:NH2	2.51	0.44
1:B:16:VAL:CG2	1:B:46:LEU:HA	2.48	0.44
1:A:532:CYS:C	1:A:534:MET:H	2.21	0.44
1:A:115:LEU:HA	1:A:115:LEU:HD12	1.73	0.44
1:A:491:LEU:HD23	1:A:491:LEU:HA	1.85	0.44
1:B:139:GLU:HG3	1:B:139:GLU:H	1.34	0.44
1:A:357:ARG:HB3	1:B:548:ARG:HH22	1.81	0.44
1:A:267:TYR:HB3	1:A:356:LEU:HD23	2.00	0.44
1:A:18:PRO:C	1:A:20:SER:H	2.22	0.44
1:B:116:SER:HB2	1:B:128:PRO:HA	1.99	0.43
1:B:416:ARG:HG3	1:B:420:MET:HE1	2.01	0.43
1:B:463:ASP:OD2	1:B:465:LYS:HG3	2.18	0.43
1:B:76:ARG:O	1:B:80:SER:HB3	2.19	0.43
1:A:509:GLU:O	1:A:510:ASN:HB2	2.18	0.43
1:B:237:PHE:CZ	1:B:241:GLU:HG3	2.53	0.43
1:A:287:VAL:CG1	1:A:288:GLU:N	2.82	0.43
1:B:22:ARG:HA	1:B:25:TRP:CE2	2.52	0.43
1:A:294:LEU:HD11	1:A:308:LEU:HD13	2.01	0.43
1:B:177:LEU:HD23	1:B:178:MET:CE	2.49	0.43
1:B:287:VAL:CG1	1:B:288:GLU:N	2.80	0.43
1:B:508:PRO:HG2	1:B:544:TYR:CE2	2.54	0.43
1:B:562:PRO:HA	1:B:563:PRO:HD3	1.93	0.43
1:A:429:LYS:HA	1:A:506:ILE:HD11	2.01	0.43
1:A:22:ARG:HA	1:A:25:TRP:CD2	2.54	0.43
1:B:16:VAL:HG21	1:B:46:LEU:HB2	2.00	0.43
1:A:395:GLN:HB2	1:A:395:GLN:HE21	1.62	0.42
1:B:160:TYR:O	1:B:163:VAL:HG22	2.17	0.42
1:B:17:LEU:HD21	1:B:23:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:THR:C	1:A:120:ILE:H	2.22	0.42
1:B:55:ILE:HG12	1:B:81:THR:HG21	2.00	0.42
1:A:22:ARG:HA	1:A:25:TRP:CE2	2.54	0.42
1:A:410:LYS:HE3	1:A:421:ASP:OD2	2.19	0.42
1:B:413:SER:HB2	1:B:414:VAL:H	1.75	0.42
1:A:457:ASP:HB3	1:A:470:MET:HE1	2.00	0.42
1:A:331:GLN:O	1:A:335:LYS:HG2	2.18	0.42
1:B:429:LYS:HA	1:B:506:ILE:HD11	2.01	0.42
1:A:69:PHE:CD2	1:A:386:PHE:HE1	2.38	0.42
1:A:47:LEU:HD21	1:A:115:LEU:HD21	2.00	0.42
1:B:330:MET:HE2	1:B:374:LYS:HE2	2.02	0.42
1:A:295:ASP:OD2	1:A:323:ARG:HD3	2.20	0.42
1:B:79:LEU:O	1:B:82:CYS:HB3	2.20	0.42
1:B:57:LEU:HD23	1:B:62:LEU:HD21	2.02	0.42
1:A:224:LEU:O	1:A:225:GLN:C	2.58	0.42
1:B:224:LEU:O	1:B:225:GLN:C	2.58	0.42
1:A:456:ASP:OD1	1:A:457:ASP:N	2.50	0.41
1:B:236:ILE:H	1:B:236:ILE:HD12	1.85	0.41
1:B:222:LYS:HB2	1:B:223:PRO:HD3	2.01	0.41
1:B:532:CYS:C	1:B:534:MET:H	2.24	0.41
1:B:456:ASP:OD1	1:B:457:ASP:N	2.49	0.41
1:B:115:LEU:HD12	1:B:115:LEU:HA	1.80	0.41
1:B:240:ILE:HD13	1:B:240:ILE:HA	1.87	0.41
1:B:118:THR:C	1:B:120:ILE:H	2.24	0.41
1:B:4:TRP:CH2	1:B:5:ARG:HD2	2.56	0.41
1:A:93:LEU:HA	1:A:111:THR:OG1	2.21	0.41
1:B:295:ASP:OD2	1:B:323:ARG:HD3	2.21	0.41
1:A:544:TYR:CD1	1:A:544:TYR:N	2.88	0.41
1:A:393:LEU:HD22	1:A:395:GLN:O	2.20	0.40
1:B:393:LEU:HD11	1:B:397:LEU:CD2	2.42	0.40
1:A:56:ASN:O	1:A:59:GLU:HB2	2.22	0.40
1:B:410:LYS:HE3	1:B:421:ASP:OD2	2.21	0.40
1:B:18:PRO:C	1:B:20:SER:H	2.24	0.40
1:A:94:PHE:CE2	1:A:108:VAL:HG13	2.56	0.40
1:A:177:LEU:HD23	1:A:178:MET:CE	2.52	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	518/587 (88%)	462 (89%)	50 (10%)	6 (1%)	16	37
1	B	531/587 (90%)	475 (90%)	47 (9%)	9 (2%)	11	27
All	All	1049/1174 (89%)	937 (89%)	97 (9%)	15 (1%)	14	33

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	ASP
1	A	123	ASN
1	B	104	ASP
1	B	123	ASN
1	B	88	LEU
1	B	457	ASP
1	A	263	ALA
1	A	533	GLN
1	B	217	GLN
1	B	263	ALA
1	B	533	GLN
1	A	88	LEU
1	A	217	GLN
1	B	467	TRP
1	B	562	PRO

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	481/529 (91%)	459 (95%)	22 (5%)	33	62
1	B	488/529 (92%)	463 (95%)	25 (5%)	29	57
All	All	969/1058 (92%)	922 (95%)	47 (5%)	31	59

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	24	THR
1	A	57	LEU
1	A	81	THR
1	A	83	CYS
1	A	93	LEU
1	A	124	ARG
1	A	189	MET
1	A	197	CYS
1	A	235	ILE
1	A	260	THR
1	A	282	ARG
1	A	294	LEU
1	A	344	VAL
1	A	347	THR
1	A	393	LEU
1	A	395	GLN
1	A	409	LEU
1	A	448	ASN
1	A	470	MET
1	A	512	THR
1	A	522	SER
1	B	22	ARG
1	B	24	THR
1	B	57	LEU
1	B	83	CYS
1	B	93	LEU
1	B	124	ARG
1	B	139	GLU
1	B	141	ILE
1	B	189	MET
1	B	197	CYS
1	B	235	ILE
1	B	260	THR
1	B	282	ARG

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Mol	Chain	Res	Type
1	B	294	LEU
1	B	344	VAL
1	B	347	THR
1	B	377	ASN
1	B	393	LEU
1	B	395	GLN
1	B	409	LEU
1	B	413	SER
1	B	448	ASN
1	B	470	MET
1	B	512	THR
1	B	522	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	GLN
1	A	348	GLN
1	A	395	GLN
1	B	231	GLN
1	B	348	GLN
1	B	395	GLN
1	B	469	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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(Å²)	Q<0.9
1	A	530/587 (90%)	0.35	31 (5%)	26	26	52, 104, 175, 216	0
1	B	541/587 (92%)	0.44	28 (5%)	31	31	53, 99, 175, 216	0
All	All	1071/1174 (91%)	0.40	59 (5%)	29	28	52, 101, 175, 216	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	266	LEU	5.6
1	B	356	LEU	5.4
1	B	348	GLN	4.2
1	B	479	ALA	4.1
1	A	157	GLU	4.1
1	B	462	ARG	4.0
1	A	474	ILE	4.0
1	A	231	GLN	3.8
1	A	261	PRO	3.8
1	B	267	TYR	3.8
1	A	221	LEU	3.8
1	B	157	GLU	3.7
1	B	350	ALA	3.6
1	B	199	LEU	3.6
1	B	263	ALA	3.5
1	A	300	ALA	3.4
1	A	414	VAL	3.3
1	A	548	ARG	3.3
1	A	308	LEU	3.0
1	A	455	ARG	2.9
1	B	270	PHE	2.9
1	B	416	ARG	2.8
1	B	227	PHE	2.7
1	B	347	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	511	ALA	2.7
1	A	260	THR	2.6
1	A	263	ALA	2.5
1	B	308	LEU	2.5
1	A	419	LYS	2.5
1	A	473	LEU	2.5
1	B	190	THR	2.5
1	B	354	GLU	2.4
1	B	237	PHE	2.4
1	B	352	GLU	2.3
1	A	417	ARG	2.3
1	A	156	ASP	2.3
1	B	197	CYS	2.3
1	A	288	GLU	2.3
1	B	221	LEU	2.2
1	A	228	LEU	2.2
1	A	352	GLU	2.2
1	B	198	CYS	2.2
1	B	260	THR	2.2
1	A	561	VAL	2.2
1	A	547	HIS	2.2
1	A	560	ARG	2.2
1	A	237	PHE	2.1
1	A	105	PHE	2.1
1	A	558	LEU	2.1
1	B	261	PRO	2.1
1	A	142	TYR	2.1
1	A	559	GLY	2.1
1	A	235	ILE	2.1
1	A	227	PHE	2.0
1	B	262	GLY	2.0
1	B	511	ALA	2.0
1	A	110	TYR	2.0
1	B	258	LEU	2.0
1	B	485	PHE	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
2	ZN	B	902	1/1	0.97	0.17	-0.76	99,99,99,99	0
2	ZN	A	902	1/1	0.93	0.09	-1.01	175,175,175,175	0
2	ZN	B	901	1/1	0.99	0.13	-1.74	117,117,117,117	0
2	ZN	A	901	1/1	0.98	0.09	-2.75	144,144,144,144	0

6.5 Other polymers (i)

There are no such residues in this entry.