Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 12:33 PM EDT

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)

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:

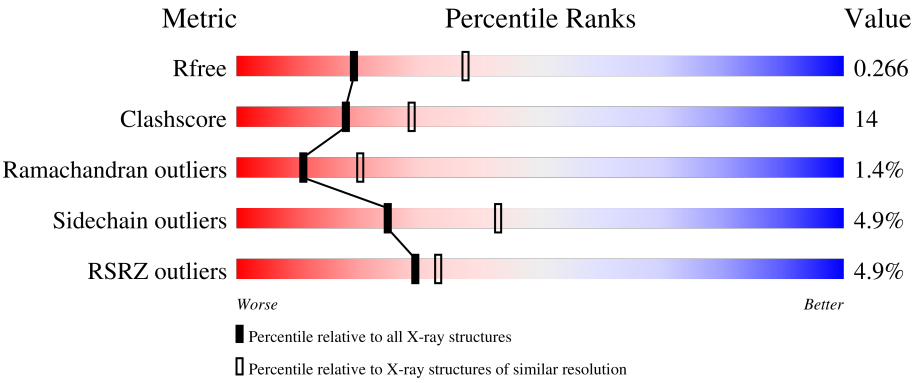
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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 <=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	4% 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).

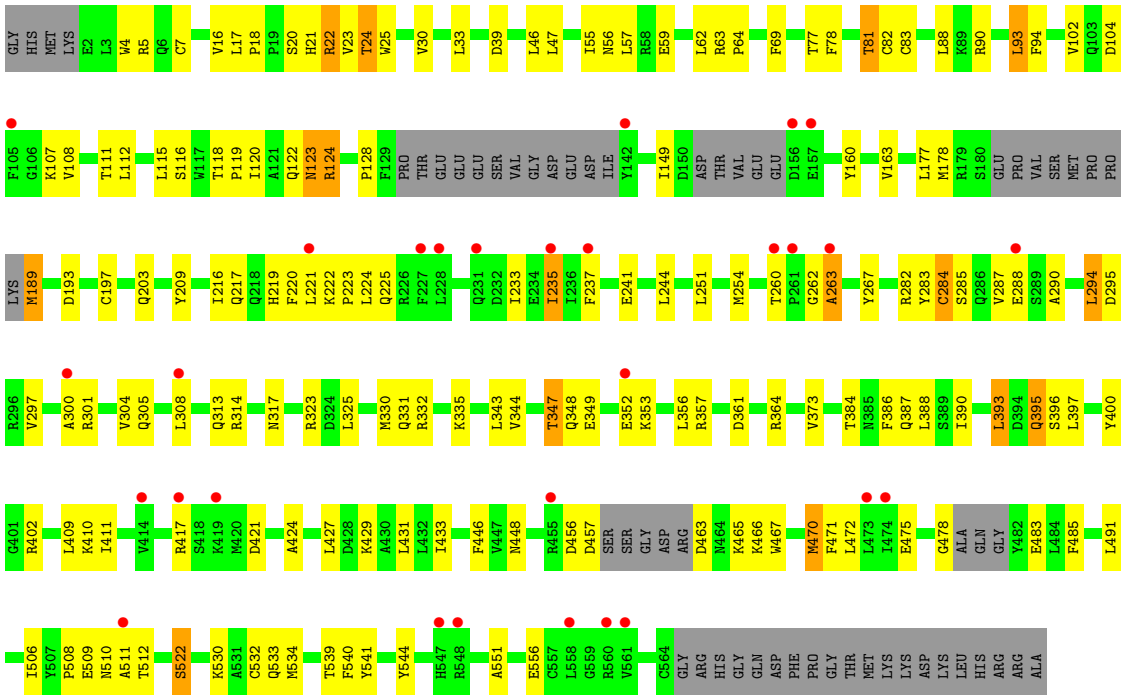
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

3 Residue-property plots (i)

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.

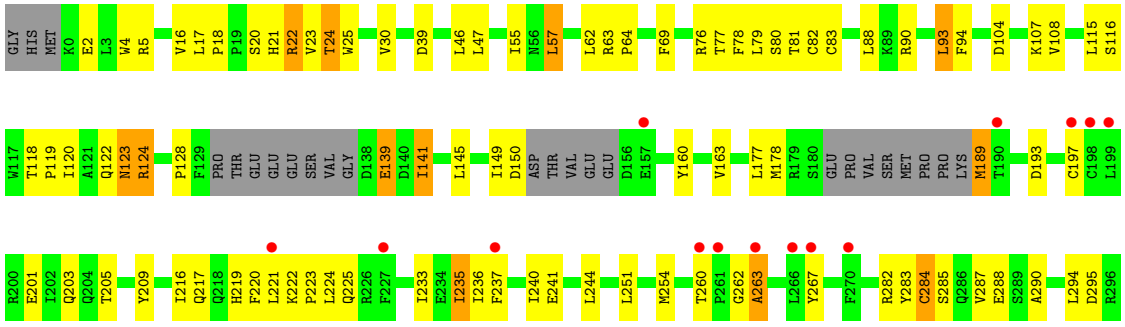
• Molecule 1: Proto-oncogene vav

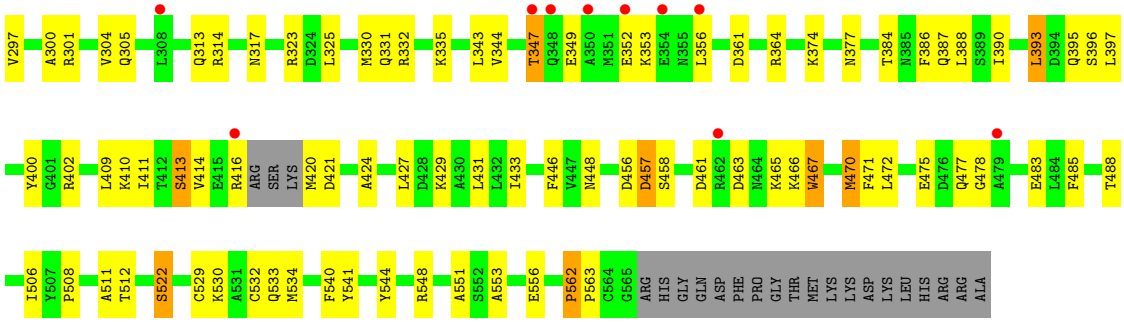
Chain A:



• Molecule 1: Proto-oncogene vav

Chain B:




V297 A300 R301 V304 Q305 L308 Q313 R314 N317 R323 D324 L325 M330 Q331 R332 K335 L343 V344 T347 Q348 E349 A350 M351 E362 K353 E354 N355 L356 D361 R364 K374 N377 T384 N385 F386 Q387 L388 S389 I390 L393 D394 Q395 S396 L397
Y400 G401 R402 L409 K410 I411 T412 S413 V414 E415 R416 ARG SER LYS M420 D421 A424 L427 D428 K429 A430 L431 L432 I433 F446 V447 N448 D456 D457 S458 D461 R462 D463 N464 K465 K466 W467 M470 F471 L472 E475 D476 Q477 G478 A479 E483 L484 F485 T488
I506 Y507 P508 A511 T512 S522 C529 K530 A531 C532 Q533 M534 F540 Y541 Y544 R548 A551 S552 A553 E556 P562 P563 G564 G565 ARG HIS GLY GLN ASP PHE PRO GLY THR MET LYS LYS ASP LYS LEU HIS ARG ARG ALA

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 ?	Depositor
R, R_{free}	0.223 , 0.271 0.223 , 0.266	Depositor DCC
R_{free} test set	1683 reflections (4.05%)	wwPDB-VP
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
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

[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

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

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:21:HIS:O	1:A:24:THR:HB	1.92	0.68
1:A:102:VAL:HG11	1:A:149:ILE:CD1	2.24	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:HA	1:A:352:GLU:OE1	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:CD	1:B:2:GLU:H	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:A:122:GLN:C	1:A:124:ARG:H	2.07	0.58
1:B:39:ASP:OD1	1:B:39:ASP:O	2.22	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:235:ILE:CG2	1:A:290:ALA:HB2	2.35	0.57
1:A:427:LEU:HD12	1:A:427:LEU:N	2.20	0.57
1:A:348:GLN:NE2	1:B:477:GLN:OE1	2.37	0.57
1:B:94:PHE:HB3	1:B:107:LYS:HG3	1.87	0.57
1:B:530:LYS:HE3	1:B:551:ALA:HA	1.86	0.57
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:386:PHE:O	1:B:390:ILE:HG13	2.05	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:A:387:GLN:OE1	1:A:396:SER:HA	2.08	0.54
1:B:149:ILE:HG22	1:B:150:ASP:N	2.21	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:A:94:PHE:HB3	1:A:107:LYS:HG3	1.90	0.53
1:B:203:GLN:HA	1:B:254:MET:CE	2.39	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:94:PHE:CD2	1:A:108:VAL:HA	2.44	0.51
1:A:235:ILE:HG21	1:A:290:ALA:HB2	1.93	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:A:39:ASP:HB2	1:A:64:PRO:HG2	1.93	0.50
1:A:116:SER:HB2	1:A:128:PRO:HA	1.93	0.50
1:A:262:GLY:O	1:A:263:ALA:HB3	2.12	0.50
1:B:352:GLU:OE1	1:B:352:GLU:CA	2.59	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:CD	1:A:556:GLU:H	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: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: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: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:209:TYR:CG	1:A:332:ARG:HG2	2.50	0.47
1:A:349:GLU:OE1	1:A:352:GLU:HG2	2.15	0.47
1:B:145:LEU:HD23	1:B:145:LEU:HA	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:A:417:ARG:HA	1:A:417:ARG:HD3	1.56	0.46
1:B:457:ASP:HB3	1:B:470:MET:HE1	1.97	0.46
1:A:361:ASP:OD1	1:A:364:ARG:NH2	2.49	0.46
1:B:216:ILE:HA	1:B:220:PHE:CD2	2.51	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:4:TRP:CH2	1:A:5:ARG:HD2	2.52	0.45
1:A:16:VAL:CG2	1:A:46:LEU:HA	2.47	0.45
1:B:544:TYR:CD1	1:B:544:TYR:N	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:A:222:LYS:HB2	1:A:223:PRO:HD3	2.00	0.44
1:B:30:VAL:HG21	1:B:141:ILE:HG21	1.99	0.44
1:B:556:GLU:CD	1:B:556:GLU:H	2.20	0.44
1:B:16:VAL:CG2	1:B:46:LEU:HA	2.48	0.44
1:B:361:ASP:OD1	1:B:364:ARG:NH2	2.51	0.44
1:A:115:LEU:HD12	1:A:115:LEU:HA	1.73	0.44
1:A:532:CYS:C	1:A:534:MET:H	2.21	0.44
1:A:491:LEU:HD23	1:A:491:LEU:HA	1.85	0.44
1:B:139:GLU:H	1:B:139:GLU:HG3	1.34	0.44
1:A:18:PRO:C	1:A:20:SER:H	2.22	0.44
1:A:267:TYR:HB3	1:A:356:LEU:HD23	2.00	0.44
1:A:357:ARG:HB3	1:B:548:ARG:HH22	1.81	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:A:509:GLU:O	1:A:510:ASN:HB2	2.18	0.43
1:B:76:ARG:O	1:B:80:SER:HB3	2.19	0.43
1:B:463:ASP:OD2	1:B:465:LYS:HG3	2.18	0.43
1:A:287:VAL:CG1	1:A:288:GLU:N	2.82	0.43
1:A:294:LEU:HD11	1:A:308:LEU:HD13	2.01	0.43
1:B:22:ARG:HA	1:B:25:TRP:CE2	2.52	0.43
1:B:177:LEU:HD23	1:B:178:MET:CE	2.49	0.43
1:B:237:PHE:CZ	1:B:241:GLU:HG3	2.53	0.43
1:A:22:ARG:HA	1:A:25:TRP:CD2	2.54	0.43
1:A:429:LYS:HA	1:A:506:ILE:HD11	2.01	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:B:16:VAL:HG21	1:B:46:LEU:HB2	2.00	0.43
1:A:395:GLN:HE21	1:A:395:GLN:HB2	1.62	0.42
1:B:17:LEU:HD21	1:B:23:VAL:HG21	2.01	0.42
1:B:160:TYR:O	1:B:163:VAL:HG22	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ARG:HA	1:A:25:TRP:CE2	2.54	0.42
1:A:118:THR:C	1:A:120:ILE:H	2.22	0.42
1:A:410:LYS:HE3	1:A:421:ASP:OD2	2.19	0.42
1:B:55:ILE:HG12	1:B:81:THR:HG21	2.00	0.42
1:B:413:SER:HB2	1:B:414:VAL:H	1.75	0.42
1:A:331:GLN:O	1:A:335:LYS:HG2	2.18	0.42
1:A:457:ASP:HB3	1:A:470:MET:HE1	2.00	0.42
1:B:429:LYS:HA	1:B:506:ILE:HD11	2.01	0.42
1:A:47:LEU:HD21	1:A:115:LEU:HD21	2.00	0.42
1:A:69:PHE:CD2	1:A:386:PHE:HE1	2.38	0.42
1:A:295:ASP:OD2	1:A:323:ARG:HD3	2.20	0.42
1:B:330:MET:HE2	1:B:374:LYS:HE2	2.02	0.42
1:A:224:LEU:O	1:A:225:GLN:C	2.58	0.42
1:B:57:LEU:HD23	1:B:62:LEU:HD21	2.02	0.42
1:B:79:LEU:O	1:B:82:CYS:HB3	2.20	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:222:LYS:HB2	1:B:223:PRO:HD3	2.01	0.41
1:B:236:ILE:HD12	1:B:236:ILE:H	1.85	0.41
1:B:532:CYS:C	1:B:534:MET:H	2.24	0.41
1:B:115:LEU:HD12	1:B:115:LEU:HA	1.80	0.41
1:B:456:ASP:OD1	1:B:457:ASP:N	2.49	0.41
1:B:240:ILE:HD13	1:B:240:ILE:HA	1.87	0.41
1:A:93:LEU:HA	1:A:111:THR:OG1	2.21	0.41
1:B:4:TRP:CH2	1:B:5:ARG:HD2	2.56	0.41
1:B:118:THR:C	1:B:120:ILE:H	2.24	0.41
1:B:295:ASP:OD2	1:B:323:ARG:HD3	2.21	0.41
1:A:544:TYR:N	1:A:544:TYR:CD1	2.88	0.41
1:A:56:ASN:O	1:A:59:GLU:HB2	2.22	0.40
1:A:393:LEU:HD22	1:A:395:GLN:O	2.20	0.40
1:B:18:PRO:C	1:B:20:SER:H	2.24	0.40
1:B:393:LEU:HD11	1:B:397:LEU:CD2	2.42	0.40
1:B:410:LYS:HE3	1:B:421:ASP:OD2	2.21	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%)	13 24
1	B	531/587 (90%)	475 (90%)	47 (9%)	9 (2%)	9 16
All	All	1049/1174 (89%)	937 (89%)	97 (9%)	15 (1%)	11 20

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%)	27 46
1	B	488/529 (92%)	463 (95%)	25 (5%)	24 41
All	All	969/1058 (92%)	922 (95%)	47 (5%)	25 43

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

Sometimes 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 (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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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

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	530/587 (90%)	0.31	29 (5%)	25	28	52, 104, 175, 216	0
1	B	541/587 (92%)	0.40	24 (4%)	34	37	53, 99, 175, 216	0
All	All	1071/1174 (91%)	0.36	53 (4%)	29	33	52, 101, 175, 216	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	266	LEU	5.5
1	B	356	LEU	5.3
1	B	348	GLN	4.1
1	A	474	ILE	4.0
1	B	479	ALA	4.0
1	A	157	GLU	4.0
1	B	462	ARG	3.9
1	A	231	GLN	3.7
1	A	221	LEU	3.7
1	A	261	PRO	3.7
1	B	267	TYR	3.7
1	B	157	GLU	3.6
1	B	350	ALA	3.5
1	B	199	LEU	3.5
1	B	263	ALA	3.4
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	2.8
1	B	416	ARG	2.7
1	B	227	PHE	2.6
1	B	347	THR	2.6

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

6.4 Ligands

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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
2	ZN	A	902	1/1	0.93	0.09	175,175,175,175	0
2	ZN	B	902	1/1	0.97	0.17	99,99,99,99	0
2	ZN	A	901	1/1	0.98	0.09	144,144,144,144	0
2	ZN	B	901	1/1	0.99	0.13	117,117,117,117	0

6.5 Other polymers

There are no such residues in this entry.