



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 12:11 PM UTC

PDB ID : 3KY9 / pdb_00003ky9
Title : Autoinhibited Vav1
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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	:	4-5-2 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

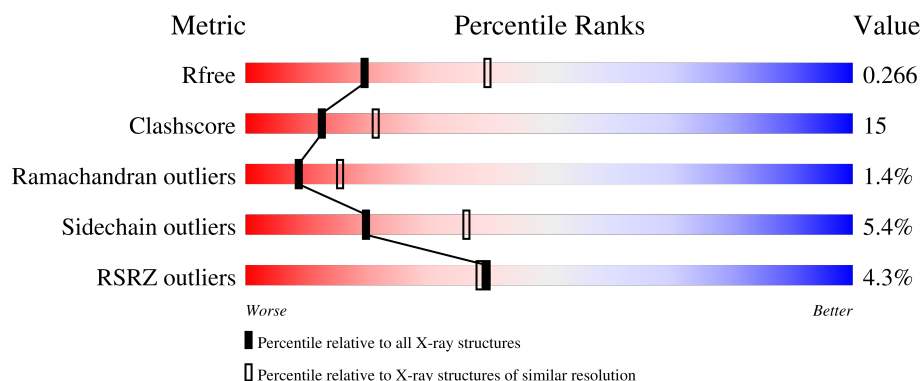
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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}	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (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 $\leq 5\%$. 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	587	3% 58% 29% 10%
1	B	587	5% 59% 28% 5% 8%

2 Entry composition

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

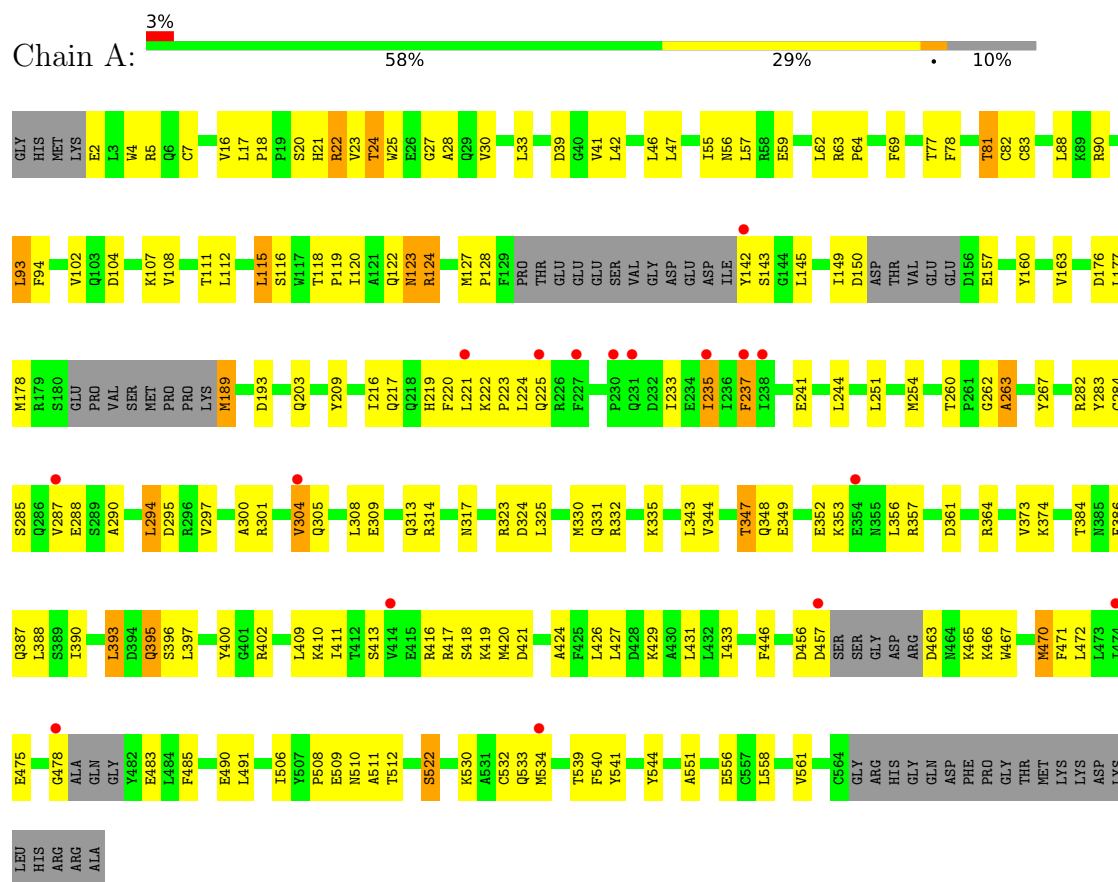
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

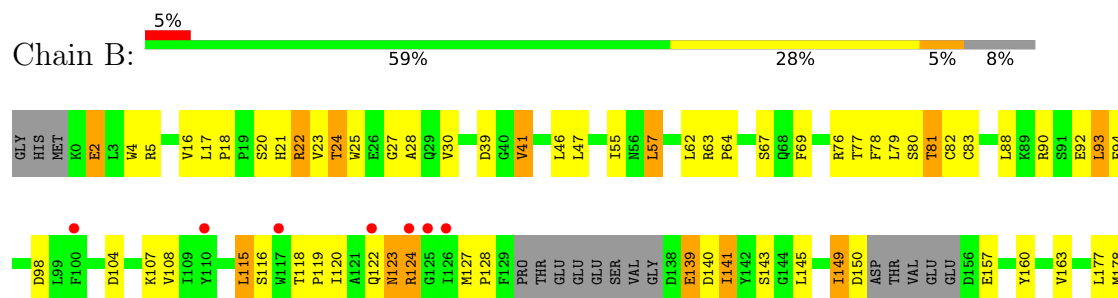
3 Residue-property plots [i](#)

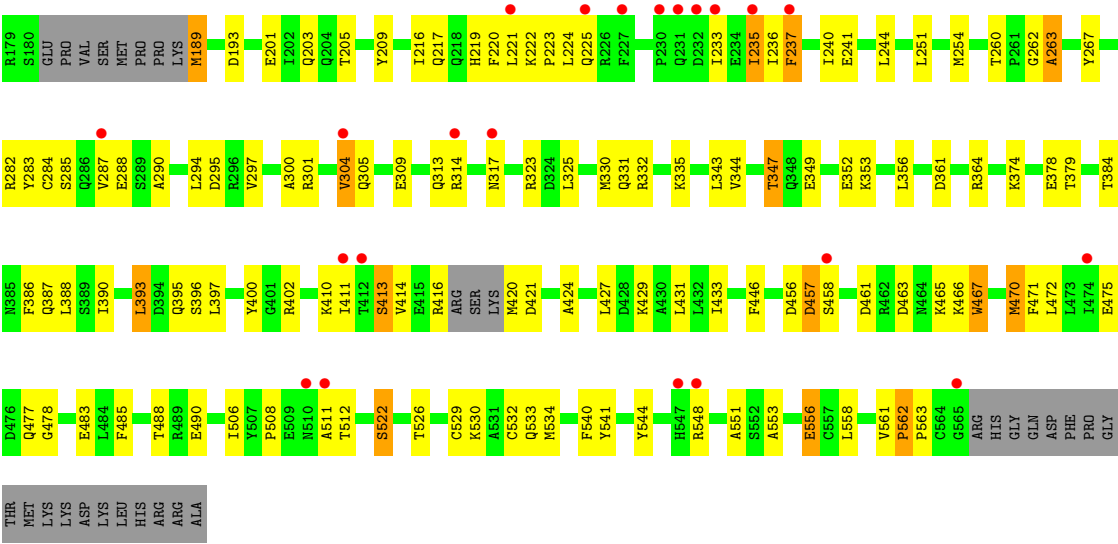
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



• Molecule 1: Proto-oncogene vav





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 , 82.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	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.*

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

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	0.51	0/4448	0.88	9/5979 (0.2%)
1	B	0.52	0/4522	0.87	13/6080 (0.2%)
All	All	0.51	0/8970	0.88	22/12059 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	MET	CA-C-N	7.96	129.03	120.11
1	A	127	MET	C-N-CA	7.96	129.03	120.11
1	B	558	LEU	N-CA-C	7.38	119.32	111.28
1	B	127	MET	CA-C-N	7.28	128.26	120.11
1	B	127	MET	C-N-CA	7.28	128.26	120.11
1	A	558	LEU	N-CA-C	7.10	119.64	111.11
1	B	561	VAL	CA-C-N	6.79	127.37	120.38
1	B	561	VAL	C-N-CA	6.79	127.37	120.38
1	A	41	VAL	N-CA-C	6.55	116.66	110.30
1	A	157	GLU	N-CA-C	-6.44	103.77	111.69
1	A	561	VAL	CA-C-N	6.44	127.01	120.38
1	A	561	VAL	C-N-CA	6.44	127.01	120.38
1	B	309	GLU	N-CA-C	-6.42	105.98	113.88
1	A	309	GLU	N-CA-C	-6.27	106.16	113.88
1	B	157	GLU	N-CA-C	-6.21	104.05	111.69
1	B	67	SER	N-CA-C	5.89	118.00	107.80
1	B	140	ASP	N-CA-C	-5.65	105.14	113.61
1	B	98	ASP	N-CA-C	-5.50	105.66	112.38
1	A	237	PHE	N-CA-C	5.35	116.80	110.97
1	B	41	VAL	N-CA-C	5.28	115.42	110.30
1	B	237	PHE	N-CA-C	5.05	116.48	111.07
1	B	92	GLU	N-CA-C	-5.05	107.10	114.12

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	137	0
1	B	4441	0	4372	137	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
All	All	8813	0	8685	267	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 (267) 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:177:LEU:HD23	1:B:178:MET:HE2	1.72	0.71
1:B:221:LEU:HD22	1:B:233:ILE:HD11	1.73	0.70
1:A:177:LEU:HD23	1:A:178:MET:HE2	1.73	0.70
1:B:21:HIS:O	1:B:24:THR:HB	1.92	0.70
1:B:2:GLU:CD	1:B:2:GLU:H	1.98	0.70
1:B:458:SER:CB	1:B:461:ASP:HB3	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:470:MET:HE1	1:B:472:LEU:HG	1.76	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: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: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
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:A:122:GLN:C	1:A:124:ARG:H	2.07	0.63
1:A:470:MET:HE1	1:A:472:LEU:HG	1.81	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:122:GLN:C	1:B:124:ARG:H	2.08	0.62
1:B:347:THR:O	1:B:353:LYS:HE2	2.00	0.61
1:B:283:TYR:C	1:B:285:SER:H	2.09	0.61
1:A:216:ILE:HA	1:A:220:PHE:HD2	1.66	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:A:283:TYR:C	1:A:285:SER:H	2.10	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:B:189:MET:HE2	1:B:189:MET:N	2.20	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:A:189:MET:N	1:A:189:MET:HE2	2.21	0.55
1:B:411:ILE:CD1	1:B:433:ILE:HD12	2.35	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:251:LEU:HD12	1:A:254:MET:HE2	1.89	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:B:416:ARG:HB2	1:B:420:MET:HE2	1.88	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:A:556:GLU:CD	1:A:556:GLU:H	2.16	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:357:ARG:HB3	1:B:548:ARG:HH12	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:203:GLN:HA	1:B:254:MET:HE1	1.92	0.51
1:B:508:PRO:HD2	1:B:511:ALA:HB2	1.91	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:297:VAL:HG12	1:B:297:VAL:O	2.10	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:A:416:ARG:HB2	1:A:420:MET:HE2	1.93	0.51
1:B:251:LEU:HD12	1:B:254:MET:HE2	1.93	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:203:GLN:HA	1:A:254:MET:HE1	1.94	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:A:466:LYS:O	1:A:467:TRP:HB2	2.10	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
1:B:287:VAL:HG13	1:B:288:GLU:HG3	1.94	0.49
1:B:556:GLU:CD	1:B:556:GLU:H	2.20	0.49
1:A:203:GLN:HA	1:A:254:MET:CE	2.42	0.49
1:A:532:CYS:C	1:A:534:MET:H	2.21	0.48
1:A:18:PRO:C	1:A:20:SER:H	2.22	0.48
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:MET:HE3	1:A:471:PHE:HA	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:118:THR:C	1:A:120:ILE:H	2.22	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:224:LEU:O	1:A:225:GLN:C	2.58	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:B:470:MET:HE3	1:B:471:PHE:HA	1.97	0.46
1:A:470:MET:HB3	1:A:485:PHE:CD1	2.50	0.46
1:B:224:LEU:O	1:B:225:GLN:C	2.58	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:B:532:CYS:C	1:B:534:MET:H	2.24	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: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
1:B:118:THR:C	1:B:120:ILE:H	2.24	0.45
1:A:216:ILE:HA	1:A:220:PHE:CD2	2.49	0.45
1:A:122:GLN:C	1:A:124:ARG:N	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:PRO:C	1:B:20:SER:H	2.24	0.45
1:A:393:LEU:HD11	1:A:397:LEU:CD2	2.42	0.45
1:A:490:GLU:H	1:A:490:GLU:CD	2.25	0.45
1:B:122:GLN:C	1:B:124:ARG:N	2.74	0.45
1:B:209:TYR:CD2	1:B:332:ARG:HG2	2.52	0.45
1:A:457:ASP:HB3	1:A:470:MET:HE2	1.99	0.44
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: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:143:SER:C	1:A:145:LEU:H	2.25	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: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:A:426:LEU:C	1:A:427:LEU:HD12	2.43	0.44
1:B:330:MET:HE2	1:B:374:LYS:HE2	2.00	0.44
1:B:116:SER:HB2	1:B:128:PRO:HA	1.99	0.43
1:B:149:ILE:O	1:B:150:ASP:C	2.60	0.43
1:A:142:TYR:O	1:A:143:SER:C	2.61	0.43
1:A:27:GLY:O	1:A:28:ALA:C	2.62	0.43
1:A:409:LEU:C	1:A:409:LEU:HD12	2.43	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:457:ASP:HB3	1:B:470:MET:HE2	2.00	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: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:490:GLU:CD	1:B:490:GLU:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:470:MET:HE3	1:A:470:MET:C	2.43	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:B:283:TYR:C	1:B:285:SER:N	2.77	0.42
1:A:295:ASP:OD2	1:A:323:ARG:HD3	2.20	0.42
1:B:470:MET:HE3	1:B:470:MET:C	2.45	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:27:GLY:O	1:B:28:ALA:C	2.63	0.42
1:B:39:ASP:C	1:B:41:VAL:H	2.28	0.42
1:B:378:GLU:O	1:B:379:THR:C	2.62	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:A:176:ASP:C	1:A:176:ASP:OD1	2.63	0.41
1:A:475:GLU:CD	1:A:478:GLY:HA3	2.45	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:143:SER:C	1:B:145:LEU:H	2.28	0.41
1:B:283:TYR:C	1:B:283:TYR:CD2	2.98	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:A:330:MET:HE2	1:A:374:LYS:HE2	2.03	0.41
1:B:4:TRP:CH2	1:B:5:ARG:HD2	2.56	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:283:TYR:C	1:A:283:TYR:CD2	3.00	0.40
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:B:410:LYS:HE3	1:B:421:ASP:OD2	2.21	0.40
1:A:149:ILE:O	1:A:150:ASP:C	2.64	0.40
1:A:418:SER:O	1:A:419:LYS:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ARG:O	1:A:324:ASP:C	2.64	0.40
1:A:94:PHE:CE2	1:A:108:VAL:HG13	2.56	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%)	10	19
1	B	531/587 (90%)	475 (90%)	47 (9%)	9 (2%)	7	12
All	All	1049/1174 (89%)	937 (89%)	97 (9%)	15 (1%)	9	15

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 ⓘ

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%)	457 (95%)	24 (5%)	22	40
1	B	488/529 (92%)	460 (94%)	28 (6%)	18	34
All	All	969/1058 (92%)	917 (95%)	52 (5%)	20	36

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	22	ARG
1	A	24	THR
1	A	42	LEU
1	A	57	LEU
1	A	81	THR
1	A	83	CYS
1	A	93	LEU
1	A	115	LEU
1	A	124	ARG
1	A	189	MET
1	A	235	ILE
1	A	260	THR
1	A	282	ARG
1	A	294	LEU
1	A	304	VAL
1	A	344	VAL
1	A	347	THR
1	A	393	LEU
1	A	395	GLN
1	A	413	SER
1	A	470	MET
1	A	512	THR
1	A	522	SER
1	B	2	GLU
1	B	22	ARG
1	B	24	THR

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Mol	Chain	Res	Type
1	B	57	LEU
1	B	81	THR
1	B	83	CYS
1	B	93	LEU
1	B	115	LEU
1	B	124	ARG
1	B	139	GLU
1	B	141	ILE
1	B	149	ILE
1	B	189	MET
1	B	235	ILE
1	B	260	THR
1	B	282	ARG
1	B	294	LEU
1	B	304	VAL
1	B	344	VAL
1	B	347	THR
1	B	393	LEU
1	B	395	GLN
1	B	413	SER
1	B	470	MET
1	B	512	THR
1	B	522	SER
1	B	526	THR
1	B	556	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	GLN
1	A	204	GLN
1	A	219	HIS
1	A	225	GLN
1	A	231	GLN
1	A	348	GLN
1	A	395	GLN
1	B	203	GLN
1	B	204	GLN
1	B	219	HIS
1	B	225	GLN
1	B	231	GLN
1	B	348	GLN

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Mol	Chain	Res	Type
1	B	395	GLN
1	B	453	GLN
1	B	469	HIS
1	B	554	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 oligosaccharides 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, 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	530/587 (90%)	0.31	17 (3%)	50 48	52, 104, 175, 216	0
1	B	541/587 (92%)	0.42	29 (5%)	31 30	53, 99, 175, 216	0
All	All	1071/1174 (91%)	0.37	46 (4%)	40 38	52, 101, 175, 216	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	548	ARG	4.5
1	A	235	ILE	3.8
1	B	235	ILE	3.6
1	B	231	GLN	3.4
1	B	237	PHE	3.4
1	B	124	ARG	3.2
1	B	547	HIS	3.1
1	A	237	PHE	3.1
1	A	231	GLN	3.1
1	A	287	VAL	3.0
1	A	221	LEU	3.0
1	A	414	VAL	3.0
1	B	565	GLY	2.8
1	B	412	THR	2.8
1	B	227	PHE	2.8
1	B	125	GLY	2.8
1	A	474	ILE	2.7
1	B	230	PRO	2.7
1	B	511	ALA	2.7
1	B	233	ILE	2.6
1	B	126	ILE	2.6
1	A	238	ILE	2.6
1	B	287	VAL	2.6
1	B	221	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	304	VAL	2.5
1	A	534	MET	2.5
1	B	232	ASP	2.5
1	A	354	GLU	2.5
1	A	225	GLN	2.4
1	B	314	ARG	2.4
1	A	230	PRO	2.4
1	B	225	GLN	2.4
1	A	142	TYR	2.3
1	B	474	ILE	2.3
1	B	117	TRP	2.2
1	B	317	ASN	2.2
1	B	110	TYR	2.1
1	A	304	VAL	2.1
1	A	227	PHE	2.1
1	B	411	ILE	2.1
1	B	510	ASN	2.1
1	A	478	GLY	2.1
1	A	457	ASP	2.0
1	B	458	SER	2.0
1	B	100	PHE	2.0
1	B	122	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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, 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	B-factors(Å ²)	Q<0.9
2	ZN	A	902	1/1	0.94	0.07	175,175,175,175	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	901	1/1	0.98	0.05	144,144,144,144	0
2	ZN	B	901	1/1	0.99	0.03	117,117,117,117	0
2	ZN	B	902	1/1	0.99	0.03	99,99,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.