



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:19 PM GMT

PDB ID : 3WVN
Title : Complex structure of VinN with L-aspartate
Authors : Miyanaga, A.; Cieslak, J.; Shinohara, Y.; Kudo, F.; Eguchi, T.
Deposited on : 2014-05-30
Resolution : 2.20 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

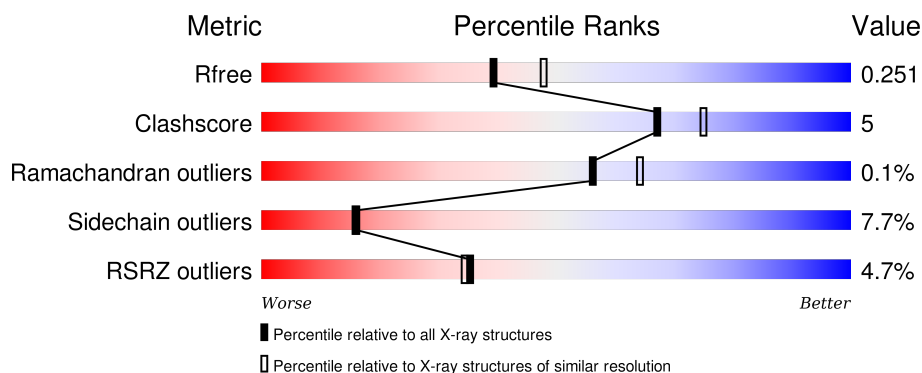
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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 $\leq 5\%$. 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	541	<div> <div>3%</div> <div> <div></div> <div>62%</div> <div>9%</div> <div>•</div> <div>28%</div> </div> </div>
1	B	541	<div> <div>3%</div> <div> <div></div> <div>57%</div> <div>6%</div> <div>••</div> <div>34%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5854 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 Non-ribosomal peptide synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			2948	1874	508	551	15			
1	B	355	Total	C	N	O	S	0	0	0
			2712	1727	469	501	15			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	EXPRESSION TAG	UNP Q76KY2
A	-14	ASN	-	EXPRESSION TAG	UNP Q76KY2
A	-13	HIS	-	EXPRESSION TAG	UNP Q76KY2
A	-12	LYS	-	EXPRESSION TAG	UNP Q76KY2
A	-11	VAL	-	EXPRESSION TAG	UNP Q76KY2
A	-10	HIS	-	EXPRESSION TAG	UNP Q76KY2
A	-9	HIS	-	EXPRESSION TAG	UNP Q76KY2
A	-8	HIS	-	EXPRESSION TAG	UNP Q76KY2
A	-7	HIS	-	EXPRESSION TAG	UNP Q76KY2
A	-6	HIS	-	EXPRESSION TAG	UNP Q76KY2
A	-5	HIS	-	EXPRESSION TAG	UNP Q76KY2
A	-4	ILE	-	EXPRESSION TAG	UNP Q76KY2
A	-3	GLU	-	EXPRESSION TAG	UNP Q76KY2
A	-2	GLY	-	EXPRESSION TAG	UNP Q76KY2
A	-1	ARG	-	EXPRESSION TAG	UNP Q76KY2
A	0	HIS	-	EXPRESSION TAG	UNP Q76KY2
A	1	MET	-	EXPRESSION TAG	UNP Q76KY2
A	2	TYR	-	EXPRESSION TAG	UNP Q76KY2
A	3	SER	-	EXPRESSION TAG	UNP Q76KY2
A	4	PRO	-	EXPRESSION TAG	UNP Q76KY2
A	5	ASP	-	EXPRESSION TAG	UNP Q76KY2
A	6	ARG	-	EXPRESSION TAG	UNP Q76KY2
A	7	ARG	-	EXPRESSION TAG	UNP Q76KY2
A	8	ALA	-	EXPRESSION TAG	UNP Q76KY2
A	9	ALA	-	EXPRESSION TAG	UNP Q76KY2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	10	LEU	-	EXPRESSION TAG	UNP Q76KY2
A	11	ASN	-	EXPRESSION TAG	UNP Q76KY2
A	12	SER	-	EXPRESSION TAG	UNP Q76KY2
A	13	VAL	-	EXPRESSION TAG	UNP Q76KY2
A	14	ALA	-	EXPRESSION TAG	UNP Q76KY2
A	15	ASN	-	EXPRESSION TAG	UNP Q76KY2
A	16	MET	-	EXPRESSION TAG	UNP Q76KY2
A	17	VAL	-	EXPRESSION TAG	UNP Q76KY2
A	18	SER	-	EXPRESSION TAG	UNP Q76KY2
A	19	ASP	-	EXPRESSION TAG	UNP Q76KY2
A	20	ASN	-	EXPRESSION TAG	UNP Q76KY2
A	21	ALA	-	EXPRESSION TAG	UNP Q76KY2
A	22	ASP	-	EXPRESSION TAG	UNP Q76KY2
A	23	LYS	-	EXPRESSION TAG	UNP Q76KY2
A	24	ASP	-	EXPRESSION TAG	UNP Q76KY2
A	25	LEU	-	EXPRESSION TAG	UNP Q76KY2
A	26	ARG	-	EXPRESSION TAG	UNP Q76KY2
A	27	TYR	-	EXPRESSION TAG	UNP Q76KY2
A	28	GLY	-	EXPRESSION TAG	UNP Q76KY2
A	29	GLY	-	EXPRESSION TAG	UNP Q76KY2
A	30	LEU	-	EXPRESSION TAG	UNP Q76KY2
A	31	VAL	-	EXPRESSION TAG	UNP Q76KY2
A	32	HIS	-	EXPRESSION TAG	UNP Q76KY2
A	33	ASP	-	EXPRESSION TAG	UNP Q76KY2
A	34	LEU	-	EXPRESSION TAG	UNP Q76KY2
A	35	LEU	-	EXPRESSION TAG	UNP Q76KY2
A	36	ALA	-	EXPRESSION TAG	UNP Q76KY2
A	37	ASP	-	EXPRESSION TAG	UNP Q76KY2
A	38	SER	-	EXPRESSION TAG	UNP Q76KY2
A	39	GLY	-	EXPRESSION TAG	UNP Q76KY2
A	40	LYS	-	EXPRESSION TAG	UNP Q76KY2
A	41	ALA	-	EXPRESSION TAG	UNP Q76KY2
A	42	THR	-	EXPRESSION TAG	UNP Q76KY2
A	43	PRO	-	EXPRESSION TAG	UNP Q76KY2
A	44	ASN	-	EXPRESSION TAG	UNP Q76KY2
A	45	SER	-	EXPRESSION TAG	UNP Q76KY2
A	46	ASP	-	EXPRESSION TAG	UNP Q76KY2
A	47	ALA	-	EXPRESSION TAG	UNP Q76KY2
B	-15	MET	-	EXPRESSION TAG	UNP Q76KY2
B	-14	ASN	-	EXPRESSION TAG	UNP Q76KY2
B	-13	HIS	-	EXPRESSION TAG	UNP Q76KY2
B	-12	LYS	-	EXPRESSION TAG	UNP Q76KY2

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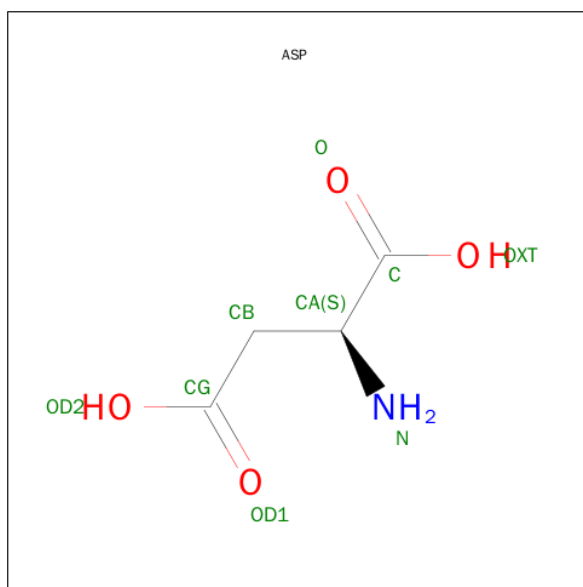
Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	VAL	-	EXPRESSION TAG	UNP Q76KY2
B	-10	HIS	-	EXPRESSION TAG	UNP Q76KY2
B	-9	HIS	-	EXPRESSION TAG	UNP Q76KY2
B	-8	HIS	-	EXPRESSION TAG	UNP Q76KY2
B	-7	HIS	-	EXPRESSION TAG	UNP Q76KY2
B	-6	HIS	-	EXPRESSION TAG	UNP Q76KY2
B	-5	HIS	-	EXPRESSION TAG	UNP Q76KY2
B	-4	ILE	-	EXPRESSION TAG	UNP Q76KY2
B	-3	GLU	-	EXPRESSION TAG	UNP Q76KY2
B	-2	GLY	-	EXPRESSION TAG	UNP Q76KY2
B	-1	ARG	-	EXPRESSION TAG	UNP Q76KY2
B	0	HIS	-	EXPRESSION TAG	UNP Q76KY2
B	1	MET	-	EXPRESSION TAG	UNP Q76KY2
B	2	TYR	-	EXPRESSION TAG	UNP Q76KY2
B	3	SER	-	EXPRESSION TAG	UNP Q76KY2
B	4	PRO	-	EXPRESSION TAG	UNP Q76KY2
B	5	ASP	-	EXPRESSION TAG	UNP Q76KY2
B	6	ARG	-	EXPRESSION TAG	UNP Q76KY2
B	7	ARG	-	EXPRESSION TAG	UNP Q76KY2
B	8	ALA	-	EXPRESSION TAG	UNP Q76KY2
B	9	ALA	-	EXPRESSION TAG	UNP Q76KY2
B	10	LEU	-	EXPRESSION TAG	UNP Q76KY2
B	11	ASN	-	EXPRESSION TAG	UNP Q76KY2
B	12	SER	-	EXPRESSION TAG	UNP Q76KY2
B	13	VAL	-	EXPRESSION TAG	UNP Q76KY2
B	14	ALA	-	EXPRESSION TAG	UNP Q76KY2
B	15	ASN	-	EXPRESSION TAG	UNP Q76KY2
B	16	MET	-	EXPRESSION TAG	UNP Q76KY2
B	17	VAL	-	EXPRESSION TAG	UNP Q76KY2
B	18	SER	-	EXPRESSION TAG	UNP Q76KY2
B	19	ASP	-	EXPRESSION TAG	UNP Q76KY2
B	20	ASN	-	EXPRESSION TAG	UNP Q76KY2
B	21	ALA	-	EXPRESSION TAG	UNP Q76KY2
B	22	ASP	-	EXPRESSION TAG	UNP Q76KY2
B	23	LYS	-	EXPRESSION TAG	UNP Q76KY2
B	24	ASP	-	EXPRESSION TAG	UNP Q76KY2
B	25	LEU	-	EXPRESSION TAG	UNP Q76KY2
B	26	ARG	-	EXPRESSION TAG	UNP Q76KY2
B	27	TYR	-	EXPRESSION TAG	UNP Q76KY2
B	28	GLY	-	EXPRESSION TAG	UNP Q76KY2
B	29	GLY	-	EXPRESSION TAG	UNP Q76KY2
B	30	LEU	-	EXPRESSION TAG	UNP Q76KY2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	31	VAL	-	EXPRESSION TAG	UNP Q76KY2
B	32	HIS	-	EXPRESSION TAG	UNP Q76KY2
B	33	ASP	-	EXPRESSION TAG	UNP Q76KY2
B	34	LEU	-	EXPRESSION TAG	UNP Q76KY2
B	35	LEU	-	EXPRESSION TAG	UNP Q76KY2
B	36	ALA	-	EXPRESSION TAG	UNP Q76KY2
B	37	ASP	-	EXPRESSION TAG	UNP Q76KY2
B	38	SER	-	EXPRESSION TAG	UNP Q76KY2
B	39	GLY	-	EXPRESSION TAG	UNP Q76KY2
B	40	LYS	-	EXPRESSION TAG	UNP Q76KY2
B	41	ALA	-	EXPRESSION TAG	UNP Q76KY2
B	42	THR	-	EXPRESSION TAG	UNP Q76KY2
B	43	PRO	-	EXPRESSION TAG	UNP Q76KY2
B	44	ASN	-	EXPRESSION TAG	UNP Q76KY2
B	45	SER	-	EXPRESSION TAG	UNP Q76KY2
B	46	ASP	-	EXPRESSION TAG	UNP Q76KY2
B	47	ALA	-	EXPRESSION TAG	UNP Q76KY2

- Molecule 2 is ASPARTIC ACID (three-letter code: ASP) (formula: $C_4H_7NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	4	1	4		
2	B	1	Total	C	N	O	0	0
			9	4	1	4		

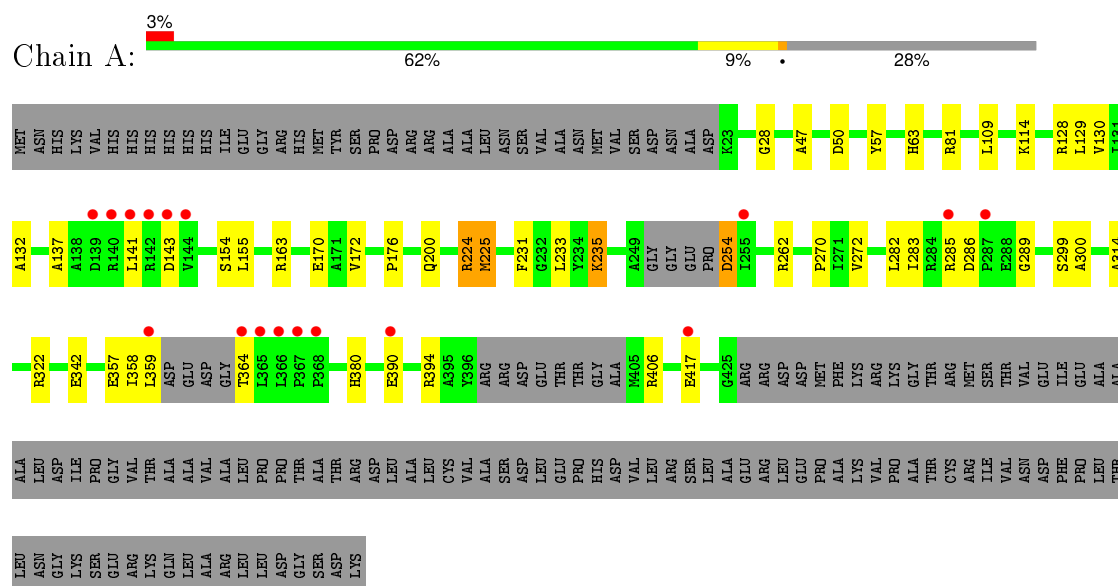
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	81	Total 81	O 81	0	0
3	B	95	Total 95	O 95	0	0

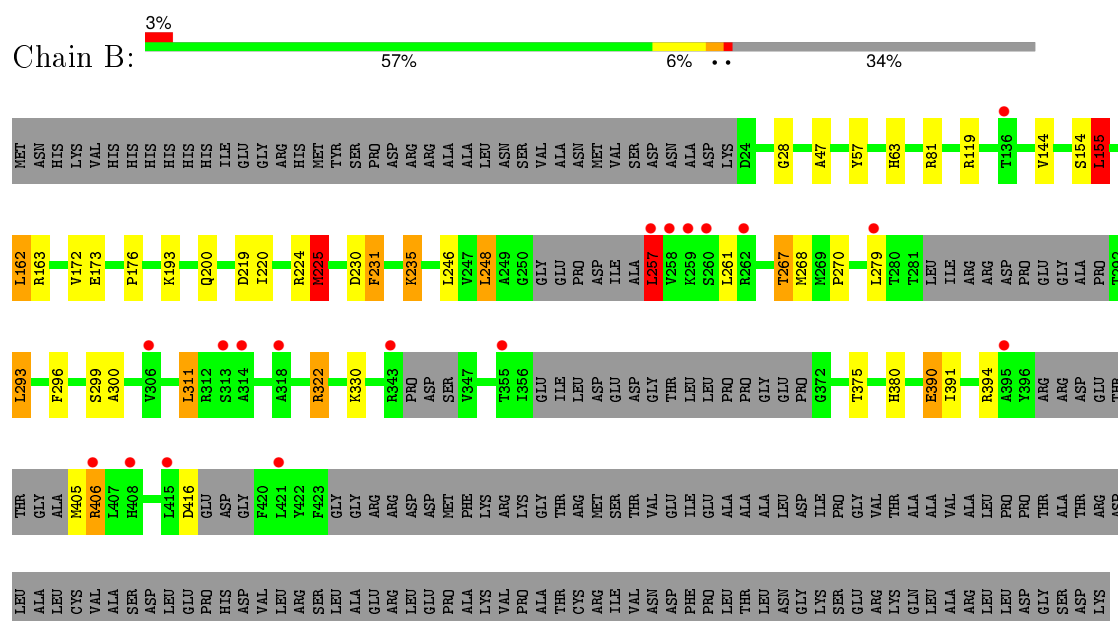
3 Residue-property plots

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: Non-ribosomal peptide synthetase



• Molecule 1: Non-ribosomal peptide synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	80.53Å 109.30Å 200.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.63 – 2.20 39.60 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.3 (39.63-2.20) 95.3 (39.60-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.207 , 0.243 0.213 , 0.251	Depositor DCC
R_{free} test set	2176 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 43056 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5854	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.75	0/3014	0.89	4/4106 (0.1%)
1	B	0.76	0/2769	0.91	9/3765 (0.2%)
All	All	0.76	0/5783	0.90	13/7871 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	B	322	ARG	NE-CZ-NH1	8.49	124.54	120.30
1	B	155	LEU	CA-CB-CG	8.44	134.72	115.30
1	B	311	LEU	CA-CB-CG	6.85	131.06	115.30
1	B	257	LEU	CA-CB-CG	6.66	130.61	115.30
1	B	322	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	B	235	LYS	CD-CE-NZ	6.36	126.33	111.70
1	A	322	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	235	LYS	CD-CE-NZ	5.69	124.79	111.70
1	A	128	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	162	LEU	CA-CB-CG	5.46	127.86	115.30
1	B	119	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	B	225	MET	CG-SD-CE	5.25	108.59	100.20

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	2948	0	2934	26	0
1	B	2712	0	2699	28	0
2	A	9	0	3	0	0
2	B	9	0	3	1	0
3	A	81	0	0	4	0
3	B	95	0	0	2	0
All	All	5854	0	5639	54	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 5.

All (54) 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:375:THR:CG2	1:B:406:ARG:HD3	2.16	0.76
1:B:375:THR:CG2	1:B:406:ARG:CD	2.74	0.65
1:B:375:THR:HG21	1:B:406:ARG:HD3	1.77	0.65
1:A:358:ILE:O	1:A:359:LEU:HD23	1.97	0.64
1:A:262:ARG:NH2	1:A:286:ASP:OD2	2.30	0.63
1:B:375:THR:HG21	1:B:406:ARG:CD	2.30	0.61
1:B:246:LEU:HG	1:B:248:LEU:HD12	1.82	0.61
1:B:225:MET:HE2	1:B:270:PRO:HB2	1.82	0.61
1:B:219:ASP:OD1	1:B:267:THR:HG21	2.01	0.59
1:A:132:ALA:HB2	1:A:141:LEU:HD22	1.85	0.59
1:B:219:ASP:HA	1:B:267:THR:HG21	1.85	0.56
1:A:224:ARG:NH2	1:A:254:ASP:OD2	2.38	0.56
1:B:193:LYS:HE3	1:B:391:ILE:HG21	1.87	0.56
1:A:63:HIS:CE1	1:A:163:ARG:HH11	2.25	0.55
1:A:225:MET:N	1:A:225:MET:HE2	2.21	0.55
1:B:28:GLY:HA2	1:B:200:GLN:HE21	1.73	0.54
1:B:246:LEU:HG	1:B:248:LEU:CD1	2.38	0.52
1:B:219:ASP:OD1	1:B:267:THR:CG2	2.58	0.51
1:A:28:GLY:HA2	1:A:200:GLN:HE21	1.75	0.51
1:A:130:VAL:HG11	1:A:141:LEU:HD23	1.93	0.50
1:B:63:HIS:CE1	1:B:163:ARG:HH11	2.30	0.50
1:B:293:LEU:HD23	1:B:296:PHE:CZ	2.47	0.49
1:B:47:ALA:HB2	1:B:57:TYR:CD1	2.47	0.49
1:A:225:MET:HE1	1:A:270:PRO:HG2	1.95	0.49
1:A:283:ILE:HG21	1:A:314:ALA:CB	2.43	0.48
1:A:137:ALA:O	1:A:141:LEU:HD13	2.14	0.48
1:A:63:HIS:HE1	3:A:715:HOH:O	1.97	0.48
1:A:50:ASP:HB2	3:A:753:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ILE:C	1:A:359:LEU:HD23	2.35	0.47
1:A:47:ALA:HB2	1:A:57:TYR:CD1	2.49	0.47
1:A:130:VAL:CG1	1:A:141:LEU:HD23	2.44	0.47
1:B:155:LEU:C	1:B:155:LEU:HD23	2.34	0.47
1:A:283:ILE:HD11	1:A:289:GLY:HA2	1.97	0.46
1:B:230:ASP:OD1	2:B:601:ASP:N	2.49	0.46
1:B:225:MET:HG3	1:B:231:PHE:HB3	1.97	0.45
1:B:300:ALA:N	3:B:715:HOH:O	2.38	0.45
1:A:63:HIS:CE1	3:A:715:HOH:O	2.69	0.45
1:A:129:LEU:HD12	1:A:129:LEU:C	2.37	0.45
1:B:220:ILE:H	1:B:267:THR:HG22	1.83	0.44
1:B:267:THR:HG23	1:B:268:MET:HG2	1.99	0.44
1:A:299:SER:O	1:A:300:ALA:HB3	2.18	0.44
1:A:143:ASP:HA	3:A:747:HOH:O	2.18	0.44
1:B:176:PRO:CB	1:B:200:GLN:HG3	2.48	0.43
1:B:299:SER:O	1:B:300:ALA:HB3	2.19	0.43
1:B:416:ASP:OD1	1:B:416:ASP:C	2.57	0.43
1:A:225:MET:N	1:A:225:MET:CE	2.82	0.42
1:A:283:ILE:HG21	1:A:314:ALA:HB2	2.01	0.42
1:B:257:LEU:C	1:B:257:LEU:HD12	2.40	0.42
1:B:390:GLU:H	1:B:390:GLU:CD	2.23	0.41
1:A:176:PRO:CB	1:A:200:GLN:HG3	2.51	0.41
1:B:322:ARG:HD3	3:B:701:HOH:O	2.21	0.41
1:A:417:GLU:H	1:A:417:GLU:CD	2.25	0.40
1:A:176:PRO:O	1:A:200:GLN:HG3	2.21	0.40
1:B:267:THR:CG2	1:B:268:MET:HG2	2.51	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	379/541 (70%)	373 (98%)	6 (2%)	0	100	100
1	B	341/541 (63%)	336 (98%)	4 (1%)	1 (0%)	46	50
All	All	720/1082 (66%)	709 (98%)	10 (1%)	1 (0%)	56	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	330	LYS

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	312/439 (71%)	289 (93%)	23 (7%)	17	17
1	B	286/439 (65%)	263 (92%)	23 (8%)	15	15
All	All	598/878 (68%)	552 (92%)	46 (8%)	16	16

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ARG
1	A	109	LEU
1	A	114	LYS
1	A	154	SER
1	A	155	LEU
1	A	170	GLU
1	A	172	VAL
1	A	224	ARG
1	A	225	MET
1	A	231	PHE
1	A	233	LEU
1	A	235	LYS
1	A	254	ASP
1	A	272	VAL
1	A	282	LEU

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Mol	Chain	Res	Type
1	A	285	ARG
1	A	342	GLU
1	A	357	GLU
1	A	364	THR
1	A	380	HIS
1	A	390	GLU
1	A	394	ARG
1	A	406	ARG
1	B	81	ARG
1	B	144	VAL
1	B	154	SER
1	B	155	LEU
1	B	162	LEU
1	B	172	VAL
1	B	173	GLU
1	B	224	ARG
1	B	225	MET
1	B	231	PHE
1	B	235	LYS
1	B	248	LEU
1	B	257	LEU
1	B	261	LEU
1	B	267	THR
1	B	279	LEU
1	B	293	LEU
1	B	311	LEU
1	B	380	HIS
1	B	390	GLU
1	B	394	ARG
1	B	405	MET
1	B	406	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	63	HIS
1	A	200	GLN
1	B	58	GLN
1	B	63	HIS
1	B	88	ASN
1	B	200	GLN

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Mol	Chain	Res	Type
1	B	210	ASN
1	B	408	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 ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ASP	A	601	-	2,8,8	0.61	0	0,10,10	0.00	-
2	ASP	B	601	-	2,8,8	0.45	0	0,10,10	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ASP	A	601	-	-	0/2/8/8	0/0/0/0
2	ASP	B	601	-	-	0/2/8/8	0/0/0/0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	ASP	1	0

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	387/541 (71%)	0.04	17 (4%) 38 37	23, 40, 67, 89	0
1	B	355/541 (65%)	0.24	18 (5%) 32 31	24, 45, 80, 96	0
All	All	742/1082 (68%)	0.14	35 (4%) 35 34	23, 42, 75, 96	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	365	LEU	5.8
1	A	144	VAL	4.5
1	B	258	VAL	4.3
1	A	367	PRO	4.2
1	A	366	LEU	4.1
1	B	415	LEU	3.8
1	B	395	ALA	3.5
1	A	359	LEU	3.4
1	B	313	SER	3.4
1	A	140	ARG	3.3
1	A	285	ARG	3.2
1	B	408	HIS	3.1
1	B	259	LYS	3.0
1	B	314	ALA	3.0
1	A	142	ARG	3.0
1	B	355	THR	2.9
1	B	262	ARG	2.8
1	A	417	GLU	2.8
1	A	364	THR	2.8
1	A	141	LEU	2.7
1	B	306	VAL	2.7
1	A	143	ASP	2.6
1	B	136	THR	2.5
1	B	260	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	279	LEU	2.5
1	B	421	LEU	2.3
1	A	139	ASP	2.3
1	B	257	LEU	2.3
1	A	287	PRO	2.2
1	A	390	GLU	2.1
1	B	318	ALA	2.1
1	A	368	PRO	2.0
1	B	343	ARG	2.0
1	B	406	ARG	2.0
1	A	255	ILE	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	ASP	A	601	9/9	0.93	0.16	0.90	33,39,45,48	0
2	ASP	B	601	9/9	0.93	0.12	0.03	40,44,51,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.