



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:26 AM UTC

PDB ID : 1VRB / pdb_00001vrb
Title : Crystal structure of Putative asparaginyl hydroxylase (2636534) from *Bacillus subtilis* at 2.60 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2005-02-18
Resolution : 2.60 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

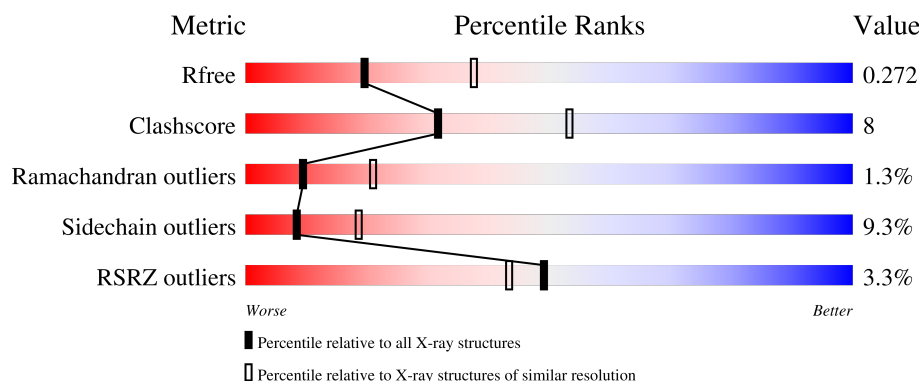
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	342	5% 67% 19% • 12%
1	B	342	2% 68% 20% • 9%
1	C	342	3% 68% 18% • 13%
1	D	342	2% 69% 19% • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9036 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 Putative asparaginyl hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	Se	0	0	0
			2223	1456	367	395	5			
1	B	311	Total	C	N	O	Se	0	0	0
			2283	1491	378	409	5			
1	C	298	Total	C	N	O	Se	0	0	0
			2210	1446	367	392	5			
1	D	313	Total	C	N	O	Se	0	0	0
			2294	1498	385	406	5			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MSE	-	expression tag	UNP P46327
A	-10	GLY	-	expression tag	UNP P46327
A	-9	SER	-	expression tag	UNP P46327
A	-8	ASP	-	expression tag	UNP P46327
A	-7	LYS	-	expression tag	UNP P46327
A	-6	ILE	-	expression tag	UNP P46327
A	-5	HIS	-	expression tag	UNP P46327
A	-4	HIS	-	expression tag	UNP P46327
A	-3	HIS	-	expression tag	UNP P46327
A	-2	HIS	-	expression tag	UNP P46327
A	-1	HIS	-	expression tag	UNP P46327
A	0	HIS	-	expression tag	UNP P46327
A	1	MSE	MET	modified residue	UNP P46327
A	18	MSE	MET	modified residue	UNP P46327
A	64	MSE	MET	modified residue	UNP P46327
A	174	MSE	MET	modified residue	UNP P46327
A	215	MSE	MET	modified residue	UNP P46327
A	248	MSE	MET	modified residue	UNP P46327
B	-11	MSE	-	expression tag	UNP P46327
B	-10	GLY	-	expression tag	UNP P46327
B	-9	SER	-	expression tag	UNP P46327

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	ASP	-	expression tag	UNP P46327
B	-7	LYS	-	expression tag	UNP P46327
B	-6	ILE	-	expression tag	UNP P46327
B	-5	HIS	-	expression tag	UNP P46327
B	-4	HIS	-	expression tag	UNP P46327
B	-3	HIS	-	expression tag	UNP P46327
B	-2	HIS	-	expression tag	UNP P46327
B	-1	HIS	-	expression tag	UNP P46327
B	0	HIS	-	expression tag	UNP P46327
B	1	MSE	MET	modified residue	UNP P46327
B	18	MSE	MET	modified residue	UNP P46327
B	64	MSE	MET	modified residue	UNP P46327
B	174	MSE	MET	modified residue	UNP P46327
B	215	MSE	MET	modified residue	UNP P46327
B	248	MSE	MET	modified residue	UNP P46327
C	-11	MSE	-	expression tag	UNP P46327
C	-10	GLY	-	expression tag	UNP P46327
C	-9	SER	-	expression tag	UNP P46327
C	-8	ASP	-	expression tag	UNP P46327
C	-7	LYS	-	expression tag	UNP P46327
C	-6	ILE	-	expression tag	UNP P46327
C	-5	HIS	-	expression tag	UNP P46327
C	-4	HIS	-	expression tag	UNP P46327
C	-3	HIS	-	expression tag	UNP P46327
C	-2	HIS	-	expression tag	UNP P46327
C	-1	HIS	-	expression tag	UNP P46327
C	0	HIS	-	expression tag	UNP P46327
C	1	MSE	MET	modified residue	UNP P46327
C	18	MSE	MET	modified residue	UNP P46327
C	64	MSE	MET	modified residue	UNP P46327
C	174	MSE	MET	modified residue	UNP P46327
C	215	MSE	MET	modified residue	UNP P46327
C	248	MSE	MET	modified residue	UNP P46327
D	-11	MSE	-	expression tag	UNP P46327
D	-10	GLY	-	expression tag	UNP P46327
D	-9	SER	-	expression tag	UNP P46327
D	-8	ASP	-	expression tag	UNP P46327
D	-7	LYS	-	expression tag	UNP P46327
D	-6	ILE	-	expression tag	UNP P46327
D	-5	HIS	-	expression tag	UNP P46327
D	-4	HIS	-	expression tag	UNP P46327
D	-3	HIS	-	expression tag	UNP P46327

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	HIS	-	expression tag	UNP P46327
D	-1	HIS	-	expression tag	UNP P46327
D	0	HIS	-	expression tag	UNP P46327
D	1	MSE	MET	modified residue	UNP P46327
D	18	MSE	MET	modified residue	UNP P46327
D	64	MSE	MET	modified residue	UNP P46327
D	174	MSE	MET	modified residue	UNP P46327
D	215	MSE	MET	modified residue	UNP P46327
D	248	MSE	MET	modified residue	UNP P46327

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0

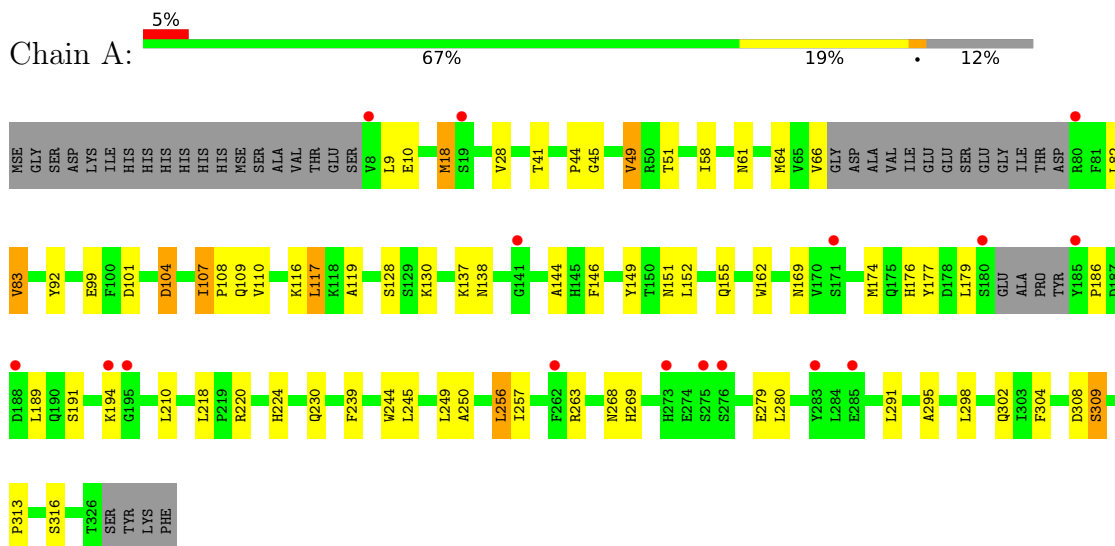
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	6	Total O 6 6	0	0
3	B	3	Total O 3 3	0	0
3	C	5	Total O 5 5	0	0
3	D	8	Total O 8 8	0	0

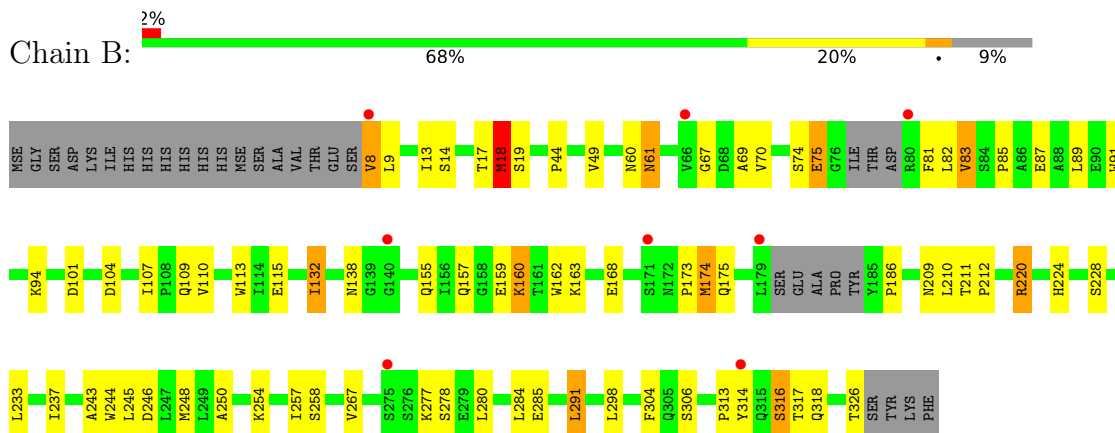
3 Residue-property plots

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.

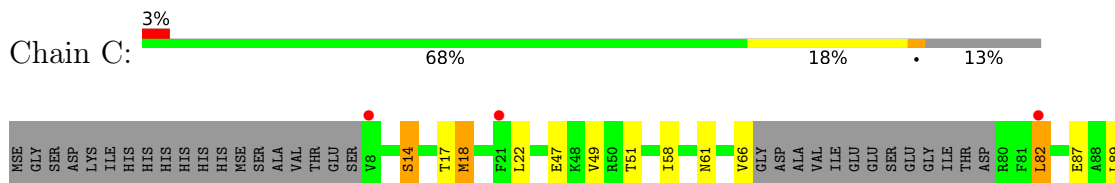
- Molecule 1: Putative asparaginyl hydroxylase

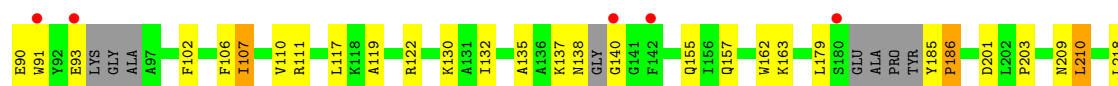


- Molecule 1: Putative asparaginyl hydroxylase



- Molecule 1: Putative asparaginyl hydroxylase





● Molecule 1: Putative asparaginyl hydroxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.30Å 104.66Å 286.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.66 – 2.60 28.66 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (28.66-2.60) 99.3 (28.66-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.221 , 0.272 0.224 , 0.272	Depositor DCC
R_{free} test set	2243 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	69.9	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 80.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9036	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: FE

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	0.98	2/2275 (0.1%)	1.07	3/3116 (0.1%)
1	B	0.97	1/2336 (0.0%)	1.02	1/3200 (0.0%)
1	C	0.90	1/2260 (0.0%)	1.02	3/3093 (0.1%)
1	D	1.06	7/2347 (0.3%)	1.09	7/3214 (0.2%)
All	All	0.98	11/9218 (0.1%)	1.05	14/12623 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	73	GLU	CA-C	11.91	1.68	1.52
1	D	70	VAL	C-O	10.19	1.35	1.24
1	C	93	GLU	C-O	9.70	1.43	1.23
1	D	74	SER	CA-CB	6.66	1.66	1.53
1	D	18	MSE	SE-CE	6.63	2.15	1.95
1	B	18	MSE	SE-CE	6.54	2.15	1.95
1	D	8	VAL	CA-CB	5.80	1.62	1.54
1	A	18	MSE	SE-CE	5.60	2.12	1.95
1	A	149	TYR	N-CA	5.10	1.52	1.45
1	D	218	LEU	N-CA	5.04	1.51	1.46
1	D	73	GLU	C-N	5.03	1.40	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	182	ALA	CA-C-N	11.06	133.67	119.84
1	D	182	ALA	C-N-CA	11.06	133.67	119.84
1	C	14	SER	CA-C-N	-8.52	111.03	119.64
1	C	14	SER	C-N-CA	-8.52	111.03	119.64
1	D	156	ILE	N-CA-C	-7.20	104.76	111.45
1	D	73	GLU	O-C-N	6.61	129.95	122.22
1	A	10	GLU	N-CA-C	-6.40	103.21	111.02
1	A	138	ASN	N-CA-C	6.27	120.79	108.18
1	D	24	GLU	N-CA-C	5.79	120.35	112.88
1	B	267	VAL	N-CA-C	5.47	115.57	108.35
1	C	179	LEU	N-CA-C	5.44	117.33	108.63
1	A	256	LEU	N-CA-C	5.42	119.52	113.01
1	D	323	GLN	N-CA-C	-5.25	105.47	111.14
1	D	81	PHE	N-CA-C	5.20	116.71	108.96

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	182	ALA	Peptide
1	D	7	SER	Peptide
1	D	80	ARG	Peptide

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	2223	0	2053	35	0
1	B	2283	0	2106	45	0
1	C	2210	0	2037	36	0
1	D	2294	0	2135	36	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	6	0	0	0	0
3	B	3	0	0	0	0
3	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	8	0	0	0	0
All	All	9036	0	8331	140	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 8.

All (140) 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:D:18:MSE:SE	1:D:18:MSE:CE	2.15	1.44
1:B:18:MSE:CE	1:B:18:MSE:SE	2.15	1.43
1:B:155:GLN:HG3	1:B:210:LEU:HB3	1.60	0.82
1:C:138:ASN:C	1:C:140:GLY:N	2.46	0.74
1:D:256:LEU:HD11	1:D:291:LEU:HD12	1.73	0.71
1:C:49:VAL:HG12	1:C:49:VAL:O	1.90	0.71
1:C:256:LEU:HD11	1:C:291:LEU:HD12	1.73	0.70
1:D:313:PRO:O	1:D:317:THR:HG23	1.93	0.69
1:B:159:GLU:HG2	1:B:211:THR:HG22	1.73	0.68
1:B:91:TRP:O	1:B:94:LYS:O	2.11	0.67
1:D:9:LEU:HD22	1:D:117:LEU:HD11	1.76	0.66
1:A:174:MSE:HG3	1:B:257:ILE:HD11	1.77	0.66
1:A:257:ILE:HD11	1:B:174:MSE:HG3	1.78	0.65
1:D:145:HIS:HB2	1:D:177:TYR:O	1.97	0.64
1:A:144:ALA:HB3	1:A:179:LEU:HD12	1.81	0.62
1:A:155:GLN:HG3	1:A:210:LEU:HB3	1.80	0.62
1:C:314:TYR:HA	1:D:317:THR:HG21	1.82	0.62
1:D:278:SER:O	1:D:280:LEU:N	2.33	0.61
1:C:313:PRO:HA	1:C:316:SER:HB2	1.82	0.60
1:B:82:LEU:O	1:B:83:VAL:HG23	2.01	0.60
1:D:176:HIS:NE2	1:D:178:ASP:CG	2.60	0.59
1:C:256:LEU:CD1	1:C:291:LEU:HD12	2.35	0.56
1:D:313:PRO:HA	1:D:316:SER:OG	2.05	0.56
1:C:261:ARG:NE	1:C:261:ARG:HA	2.20	0.56
1:A:45:GLY:HA3	1:A:107:ILE:HG21	1.88	0.56
1:C:162:TRP:NE1	1:C:210:LEU:HD22	2.20	0.56
1:B:254:LYS:O	1:B:257:ILE:HG22	2.07	0.55
1:B:314:TYR:CE1	1:B:318:GLN:NE2	2.77	0.53
1:C:130:LYS:HE3	1:C:132:ILE:HD11	1.89	0.53
1:D:45:GLY:HA3	1:D:107:ILE:HG21	1.91	0.53
1:B:87:GLU:O	1:B:91:TRP:HD1	1.92	0.53
1:C:155:GLN:HG3	1:C:210:LEU:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:PRO:O	1:A:110:VAL:HG12	2.08	0.53
1:C:117:LEU:HD23	1:C:239:PHE:HZ	1.74	0.53
1:C:257:ILE:HD11	1:D:174:MSE:HG3	1.91	0.53
1:C:324:LEU:HD13	1:D:64:MSE:HE1	1.91	0.52
1:B:313:PRO:HA	1:B:316:SER:HB2	1.91	0.52
1:C:218:LEU:HD21	1:C:224:HIS:CE1	2.45	0.52
1:D:130:LYS:HE3	1:D:132:ILE:HD11	1.90	0.52
1:A:9:LEU:HD23	1:A:18:MSE:HE1	1.91	0.52
1:A:256:LEU:HD11	1:A:291:LEU:CD1	2.40	0.51
1:A:104:ASP:OD1	1:A:104:ASP:N	2.44	0.51
1:C:89:LEU:C	1:C:91:TRP:H	2.19	0.51
1:A:49:VAL:CG1	1:A:49:VAL:O	2.59	0.51
1:B:243:ALA:O	1:B:246:ASP:HB2	2.10	0.51
1:A:291:LEU:HD22	1:B:248:MSE:HE2	1.93	0.50
1:A:176:HIS:CG	1:A:177:TYR:N	2.79	0.50
1:B:60:ASN:ND2	1:B:326:THR:C	2.70	0.50
1:D:9:LEU:HD23	1:D:18:MSE:HE1	1.93	0.50
1:C:17:THR:O	1:C:18:MSE:HB2	2.12	0.50
1:C:117:LEU:HD23	1:C:239:PHE:CZ	2.47	0.50
1:A:92:TYR:CE1	1:A:137:LYS:HB2	2.47	0.49
1:A:116:LYS:O	1:A:119:ALA:HB3	2.12	0.49
1:C:106:PHE:C	1:C:107:ILE:HG13	2.36	0.49
1:C:185:TYR:O	1:C:186:PRO:C	2.56	0.49
1:A:218:LEU:HD21	1:A:224:HIS:ND1	2.27	0.49
1:A:295:ALA:HB1	1:B:291:LEU:HD23	1.95	0.48
1:B:101:ASP:HA	1:B:132:ILE:HG23	1.95	0.48
1:C:163:LYS:HE2	1:C:201:ASP:O	2.13	0.48
1:D:139:GLY:HA2	1:D:228:SER:O	2.13	0.48
1:D:255:LYS:HE2	1:D:294:ASN:O	2.14	0.48
1:D:46:PHE:O	1:D:47:GLU:C	2.56	0.48
1:C:137:LYS:HA	1:C:231:ALA:HA	1.95	0.48
1:B:49:VAL:O	1:B:49:VAL:HG12	2.14	0.47
1:A:298:LEU:HD12	1:A:302:GLN:OE1	2.14	0.47
1:D:117:LEU:HD21	1:D:152:LEU:CD1	2.44	0.47
1:D:256:LEU:HD11	1:D:291:LEU:CD1	2.44	0.47
1:C:261:ARG:HA	1:C:261:ARG:HE	1.79	0.47
1:D:164:LEU:O	1:D:205:ALA:HB1	2.15	0.47
1:C:102:PHE:CD1	1:C:319:LEU:HD13	2.49	0.47
1:D:84:SER:OG	1:D:85:PRO:HD2	2.14	0.47
1:B:60:ASN:HD21	1:B:326:THR:C	2.23	0.46
1:A:280:LEU:HD23	1:A:280:LEU:HA	1.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:PRO:HB2	1:B:109:GLN:HB3	1.97	0.46
1:C:119:ALA:O	1:C:122:ARG:N	2.43	0.46
1:A:101:ASP:OD1	1:A:130:LYS:HD2	2.15	0.46
1:D:175:GLN:NE2	1:D:188:ASP:HB2	2.31	0.46
1:A:313:PRO:HA	1:A:316:SER:OG	2.15	0.46
1:D:13:ILE:O	1:D:14:SER:C	2.59	0.46
1:A:82:LEU:O	1:A:83:VAL:HG23	2.16	0.46
1:A:162:TRP:NE1	1:A:210:LEU:HD22	2.31	0.46
1:B:87:GLU:O	1:B:91:TRP:CD1	2.69	0.46
1:B:277:LYS:O	1:B:278:SER:C	2.57	0.46
1:A:108:PRO:O	1:A:109:GLN:C	2.60	0.45
1:A:146:PHE:CD1	1:A:146:PHE:C	2.94	0.45
1:B:173:PRO:HG2	1:B:220:ARG:HD3	1.97	0.45
1:B:160:LYS:HG3	1:B:228:SER:HB2	1.97	0.45
1:D:9:LEU:HD22	1:D:117:LEU:CD1	2.44	0.45
1:B:104:ASP:N	1:B:104:ASP:OD1	2.49	0.45
1:D:37:VAL:O	1:D:38:GLU:C	2.60	0.45
1:A:218:LEU:HD21	1:A:224:HIS:CE1	2.52	0.45
1:C:135:ALA:HB2	1:C:233:LEU:HD12	1.99	0.45
1:B:13:ILE:O	1:B:14:SER:C	2.61	0.44
1:B:17:THR:O	1:B:18:MSE:HB2	2.18	0.44
1:B:157:GLN:HB2	1:B:233:LEU:HB3	2.01	0.43
1:B:162:TRP:NE1	1:B:210:LEU:HD22	2.33	0.43
1:C:49:VAL:O	1:C:49:VAL:CG1	2.62	0.43
1:A:117:LEU:HD22	1:A:239:PHE:CZ	2.52	0.43
1:B:8:VAL:HG12	1:B:9:LEU:N	2.34	0.43
1:B:277:LYS:O	1:B:280:LEU:N	2.42	0.43
1:B:61:ASN:O	1:B:85:PRO:HG3	2.18	0.43
1:A:64:MSE:HB3	1:A:99:GLU:HB3	1.99	0.43
1:A:269:HIS:CE1	1:B:304:PHE:HB3	2.54	0.43
1:B:211:THR:O	1:B:212:PRO:C	2.59	0.43
1:D:299:THR:HG23	1:D:302:GLN:NE2	2.33	0.43
1:B:209:ASN:HB2	1:C:203:PRO:HB2	2.01	0.42
1:D:259:ASP:OD1	1:D:261:ARG:HD3	2.20	0.42
1:D:38:GLU:O	1:D:41:THR:OG1	2.28	0.42
1:A:308:ASP:C	1:A:309:SER:O	2.63	0.42
1:C:47:GLU:C	1:C:49:VAL:H	2.26	0.42
1:D:218:LEU:HD21	1:D:224:HIS:CE1	2.55	0.42
1:A:268:ASN:OD1	1:A:268:ASN:C	2.62	0.42
1:B:107:ILE:O	1:B:110:VAL:HG12	2.20	0.42
1:B:250:ALA:HB3	1:B:306:SER:OG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:GLN:HE21	1:D:188:ASP:HB2	1.84	0.41
1:D:298:LEU:HD12	1:D:298:LEU:HA	1.90	0.41
1:B:113:TRP:HZ3	1:B:237:ILE:HD12	1.84	0.41
1:B:163:LYS:O	1:B:224:HIS:HA	2.20	0.41
1:C:313:PRO:HA	1:C:316:SER:CB	2.50	0.41
1:B:284:LEU:O	1:B:285:GLU:C	2.63	0.41
1:C:304:PHE:O	1:C:307:GLN:HG2	2.20	0.41
1:C:264:GLU:OE1	1:C:283:TYR:OH	2.35	0.41
1:B:74:SER:O	1:B:75:GLU:C	2.63	0.41
1:C:87:GLU:O	1:C:91:TRP:CD1	2.74	0.41
1:A:169:ASN:HA	1:A:194:LYS:O	2.20	0.41
1:A:244:TRP:O	1:A:245:LEU:C	2.63	0.41
1:A:249:LEU:O	1:A:250:ALA:C	2.64	0.41
1:B:211:THR:HB	1:B:212:PRO:CD	2.51	0.41
1:C:66:VAL:O	1:C:66:VAL:HG12	2.21	0.41
1:C:314:TYR:HD1	1:D:317:THR:HG22	1.85	0.41
1:A:263:ARG:HG2	1:B:174:MSE:HE2	2.03	0.41
1:A:304:PHE:CZ	1:B:280:LEU:HD23	2.55	0.41
1:D:124:PRO:HG2	1:D:242:PRO:HG2	2.03	0.41
1:B:67:GLY:C	1:B:69:ALA:N	2.79	0.40
1:D:278:SER:O	1:D:281:ASN:N	2.53	0.40
1:C:17:THR:OG1	1:C:18:MSE:N	2.54	0.40
1:C:82:LEU:HD12	1:C:82:LEU:HA	1.96	0.40
1:D:50:ARG:HA	1:D:156:ILE:HG21	2.03	0.40
1:D:64:MSE:HB3	1:D:99:GLU:HB3	2.03	0.40
1:B:244:TRP:O	1:B:245:LEU:C	2.65	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	296/342 (86%)	275 (93%)	18 (6%)	3 (1%)	12	28
1	B	305/342 (89%)	280 (92%)	21 (7%)	4 (1%)	9	21
1	C	288/342 (84%)	266 (92%)	18 (6%)	4 (1%)	9	19
1	D	307/342 (90%)	281 (92%)	21 (7%)	5 (2%)	7	16
All	All	1196/1368 (87%)	1102 (92%)	78 (6%)	16 (1%)	9	21

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	PRO
1	B	18	MSE
1	B	75	GLU
1	C	14	SER
1	C	18	MSE
1	D	183	PRO
1	A	309	SER
1	C	90	GLU
1	D	278	SER
1	D	279	GLU
1	D	186	PRO
1	A	41	THR
1	C	186	PRO
1	D	8	VAL
1	B	186	PRO
1	B	70	VAL

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	205/294 (70%)	187 (91%)	18 (9%)	9	21
1	B	212/294 (72%)	193 (91%)	19 (9%)	9	20
1	C	206/294 (70%)	186 (90%)	20 (10%)	8	17
1	D	213/294 (72%)	192 (90%)	21 (10%)	7	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	836/1176 (71%)	758 (91%)	78 (9%)	8 18

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	VAL
1	A	49	VAL
1	A	51	THR
1	A	58	ILE
1	A	61	ASN
1	A	66	VAL
1	A	83	VAL
1	A	104	ASP
1	A	107	ILE
1	A	117	LEU
1	A	128	SER
1	A	151	ASN
1	A	152	LEU
1	A	189	LEU
1	A	191	SER
1	A	220	ARG
1	A	230	GLN
1	A	279	GLU
1	B	8	VAL
1	B	19	SER
1	B	61	ASN
1	B	81	PHE
1	B	83	VAL
1	B	89	LEU
1	B	115	GLU
1	B	132	ILE
1	B	138	ASN
1	B	160	LYS
1	B	168	GLU
1	B	174	MSE
1	B	175	GLN
1	B	220	ARG
1	B	258	SER
1	B	291	LEU
1	B	298	LEU
1	B	316	SER
1	B	317	THR

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Mol	Chain	Res	Type
1	C	22	LEU
1	C	51	THR
1	C	58	ILE
1	C	61	ASN
1	C	82	LEU
1	C	107	ILE
1	C	110	VAL
1	C	111	ARG
1	C	157	GLN
1	C	209	ASN
1	C	210	LEU
1	C	220	ARG
1	C	232	THR
1	C	253	ARG
1	C	258	SER
1	C	267	VAL
1	C	271	SER
1	C	287	LEU
1	C	316	SER
1	C	318	GLN
1	D	8	VAL
1	D	9	LEU
1	D	27	PRO
1	D	49	VAL
1	D	51	THR
1	D	52	LEU
1	D	58	ILE
1	D	61	ASN
1	D	84	SER
1	D	89	LEU
1	D	107	ILE
1	D	111	ARG
1	D	157	GLN
1	D	164	LEU
1	D	175	GLN
1	D	189	LEU
1	D	206	GLU
1	D	220	ARG
1	D	280	LEU
1	D	306	SER
1	D	317	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	157	GLN
1	A	169	ASN
1	B	60	ASN
1	B	138	ASN
1	B	155	GLN
1	B	157	GLN
1	B	230	GLN
1	B	294	ASN
1	C	157	GLN
1	C	169	ASN
1	C	260	ASN
1	C	269	HIS
1	C	270	GLN
1	C	294	ASN
1	C	307	GLN
1	D	155	GLN
1	D	172	ASN
1	D	268	ASN
1	D	294	ASN

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	297/342 (86%)	0.39	16 (5%) 31 26	59, 67, 76, 83	0
1	B	306/342 (89%)	0.21	8 (2%) 57 51	59, 67, 75, 87	0
1	C	293/342 (85%)	0.46	10 (3%) 48 42	60, 67, 76, 84	0
1	D	308/342 (90%)	0.31	6 (1%) 66 61	58, 67, 76, 91	0
All	All	1204/1368 (88%)	0.34	40 (3%) 49 43	58, 67, 76, 91	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	180	SER	4.7
1	D	74	SER	4.6
1	D	79	ASP	3.9
1	A	80	ARG	3.6
1	B	80	ARG	3.5
1	B	8	VAL	3.3
1	A	180	SER	3.2
1	A	195	GLY	3.1
1	C	142	PHE	3.1
1	C	267	VAL	3.1
1	A	8	VAL	3.1
1	A	275	SER	3.0
1	C	140	GLY	3.0
1	D	275	SER	2.8
1	C	93	GLU	2.8
1	A	188	ASP	2.7
1	D	66	VAL	2.7
1	A	285	GLU	2.6
1	B	66	VAL	2.6
1	B	140	GLY	2.5
1	C	8	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	171	SER	2.4
1	D	7	SER	2.4
1	A	185	TYR	2.4
1	C	275	SER	2.4
1	A	276	SER	2.4
1	A	141	GLY	2.4
1	C	91	TRP	2.3
1	D	67	GLY	2.3
1	B	179	LEU	2.3
1	A	283	TYR	2.2
1	B	314	TYR	2.1
1	B	171	SER	2.1
1	A	19	SER	2.1
1	C	21	PHE	2.1
1	A	194	LYS	2.1
1	A	262	PHE	2.0
1	B	275	SER	2.0
1	C	82	LEU	2.0
1	A	273	HIS	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($\text{\AA}^2$)	Q<0.9
2	FE	B	555	1/1	0.87	0.10	104,104,104,104	0
2	FE	C	555	1/1	0.89	0.08	104,104,104,104	0
2	FE	D	555	1/1	0.91	0.14	85,85,85,85	0
2	FE	A	555	1/1	0.92	0.07	104,104,104,104	0

6.5 Other polymers [i](#)

There are no such residues in this entry.