



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:29 AM UTC

PDB ID : 5EFV / pdb_00005efv
Title : The host-recognition device of Staphylococcus aureus phage Phi11
Authors : Koc, C.; Kuhner, P.; Xia, G.; Spinelli, S.; Roussel, A.; Cambillau, C.; Stehle, T.
Deposited on : 2015-10-26
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

<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

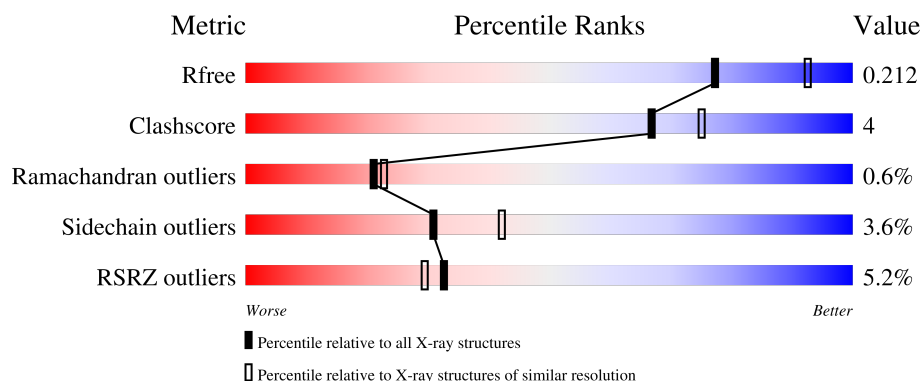
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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	648	9% 87% 9% ..
1	B	648	3% 86% 11% ..
1	C	648	3% 87% 9% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16771 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 Phi ETA orf 56-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	631	Total	C	N	O	S	0	0	0
			5025	3207	845	957	16			
1	B	635	Total	C	N	O	S	0	0	0
			5167	3287	885	980	15			
1	C	630	Total	C	N	O	S	0	0	0
			5132	3265	883	969	15			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	HIS	-	expression tag	UNP Q8SDT4
A	-10	HIS	-	expression tag	UNP Q8SDT4
A	-9	HIS	-	expression tag	UNP Q8SDT4
A	-8	HIS	-	expression tag	UNP Q8SDT4
A	-7	HIS	-	expression tag	UNP Q8SDT4
A	-6	HIS	-	expression tag	UNP Q8SDT4
A	-5	LEU	-	expression tag	UNP Q8SDT4
A	-4	VAL	-	expression tag	UNP Q8SDT4
A	-3	PRO	-	expression tag	UNP Q8SDT4
A	-2	ARG	-	expression tag	UNP Q8SDT4
A	-1	GLY	-	expression tag	UNP Q8SDT4
A	0	SER	-	expression tag	UNP Q8SDT4
B	-11	HIS	-	expression tag	UNP Q8SDT4
B	-10	HIS	-	expression tag	UNP Q8SDT4
B	-9	HIS	-	expression tag	UNP Q8SDT4
B	-8	HIS	-	expression tag	UNP Q8SDT4
B	-7	HIS	-	expression tag	UNP Q8SDT4
B	-6	HIS	-	expression tag	UNP Q8SDT4
B	-5	LEU	-	expression tag	UNP Q8SDT4
B	-4	VAL	-	expression tag	UNP Q8SDT4
B	-3	PRO	-	expression tag	UNP Q8SDT4
B	-2	ARG	-	expression tag	UNP Q8SDT4
B	-1	GLY	-	expression tag	UNP Q8SDT4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP Q8SDT4
C	-11	HIS	-	expression tag	UNP Q8SDT4
C	-10	HIS	-	expression tag	UNP Q8SDT4
C	-9	HIS	-	expression tag	UNP Q8SDT4
C	-8	HIS	-	expression tag	UNP Q8SDT4
C	-7	HIS	-	expression tag	UNP Q8SDT4
C	-6	HIS	-	expression tag	UNP Q8SDT4
C	-5	LEU	-	expression tag	UNP Q8SDT4
C	-4	VAL	-	expression tag	UNP Q8SDT4
C	-3	PRO	-	expression tag	UNP Q8SDT4
C	-2	ARG	-	expression tag	UNP Q8SDT4
C	-1	GLY	-	expression tag	UNP Q8SDT4
C	0	SER	-	expression tag	UNP Q8SDT4

- 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

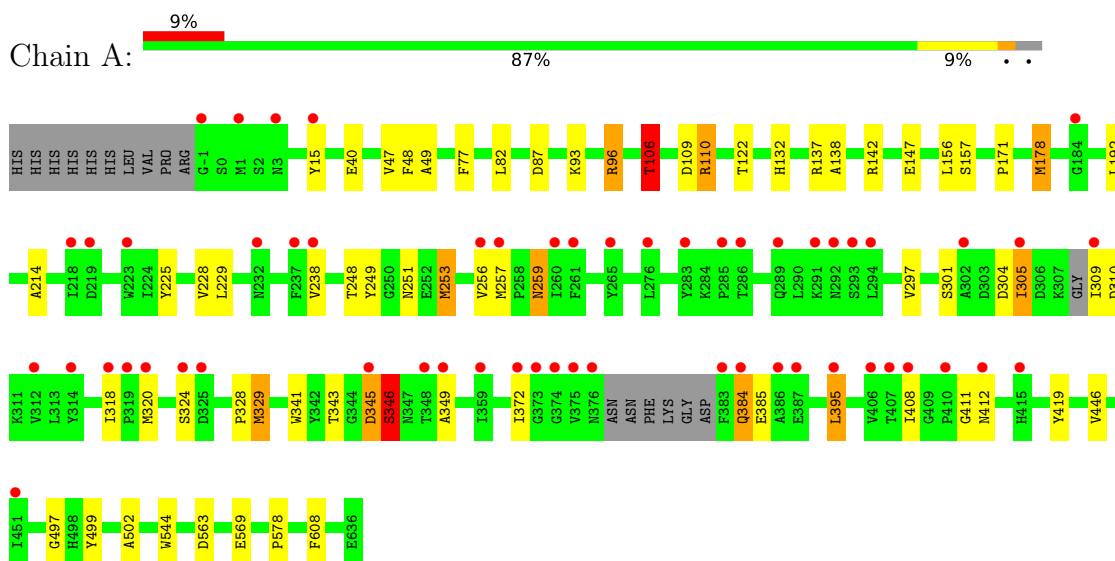
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	405	Total O 405 405	0	0
3	B	565	Total O 565 565	0	0
3	C	476	Total O 476 476	0	0

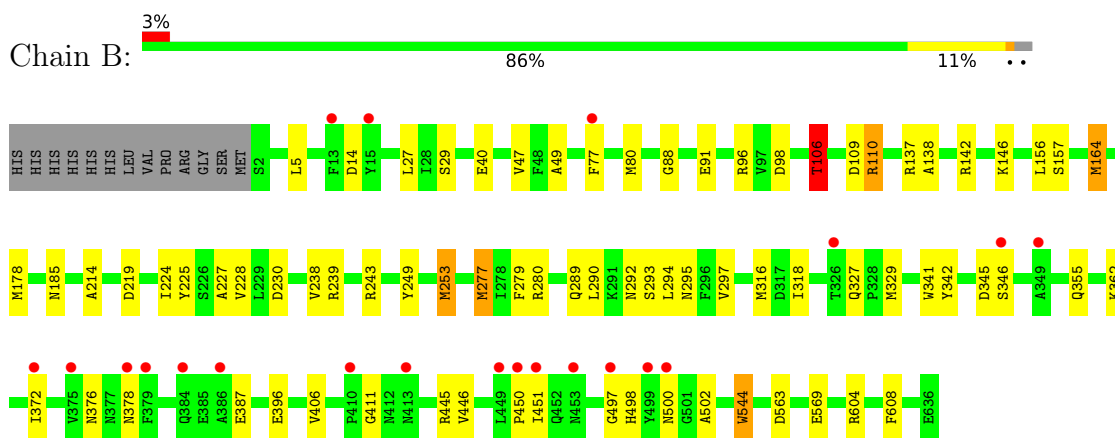
3 Residue-property plots [i](#)

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.

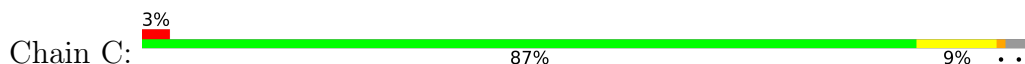
- Molecule 1: Phi ETA orf 56-like protein

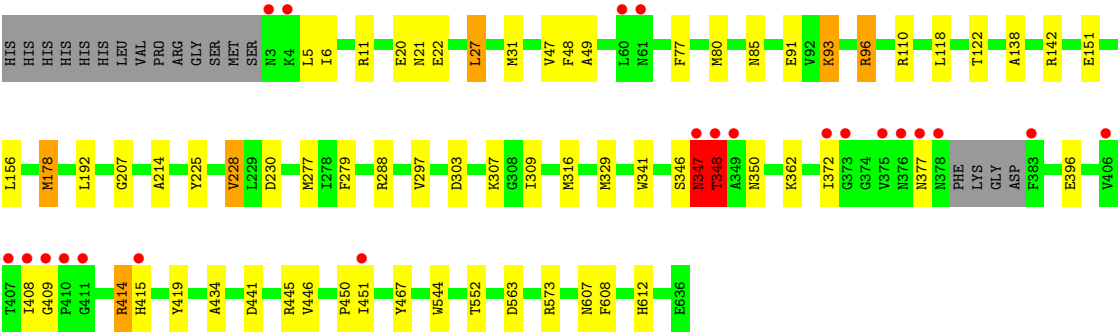


- Molecule 1: Phi ETA orf 56-like protein



- Molecule 1: Phi ETA orf 56-like protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	87.06Å 89.01Å 93.26Å 93.02° 105.25° 117.58°	Depositor
Resolution (Å)	44.40 – 2.20 44.40 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.9 (44.40-2.20) 97.9 (44.40-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.173 , 0.211 0.174 , 0.212	Depositor DCC
R_{free} test set	5827 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16771	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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	0.84	2/5152 (0.0%)	1.24	21/6996 (0.3%)
1	B	0.85	3/5298 (0.1%)	1.21	16/7178 (0.2%)
1	C	0.82	1/5260 (0.0%)	1.20	15/7124 (0.2%)
All	All	0.83	6/15710 (0.0%)	1.22	52/21298 (0.2%)

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	A	1	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	253	MET	SD-CE	-13.14	1.46	1.79
1	C	178	MET	SD-CE	-11.73	1.50	1.79
1	A	178	MET	SD-CE	-11.71	1.50	1.79
1	B	164	MET	SD-CE	-11.31	1.51	1.79
1	A	329	MET	SD-CE	-6.06	1.64	1.79
1	B	277	MET	SD-CE	-5.68	1.65	1.79

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	378	ASN	CA-C-N	9.93	139.57	121.70
1	B	378	ASN	C-N-CA	9.93	139.57	121.70
1	C	347	ASN	CA-C-N	9.58	139.83	121.54
1	C	347	ASN	C-N-CA	9.58	139.83	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	47	VAL	CA-C-N	9.18	139.07	121.54
1	C	47	VAL	C-N-CA	9.18	139.07	121.54
1	A	47	VAL	N-CA-CB	9.10	122.79	111.41
1	A	346	SER	CA-C-N	8.23	136.52	121.70
1	A	346	SER	C-N-CA	8.23	136.52	121.70
1	B	47	VAL	CA-C-N	8.05	136.92	121.54
1	B	47	VAL	C-N-CA	8.05	136.92	121.54
1	B	378	ASN	N-CA-C	8.00	122.42	111.54
1	A	47	VAL	CA-C-N	7.20	135.28	121.54
1	A	47	VAL	C-N-CA	7.20	135.28	121.54
1	C	47	VAL	N-CA-CB	7.01	120.51	111.67
1	B	563	ASP	CA-CB-CG	6.88	119.48	112.60
1	A	15	TYR	CA-C-N	6.53	128.93	120.44
1	A	15	TYR	C-N-CA	6.53	128.93	120.44
1	A	259	ASN	CA-CB-CG	6.42	119.02	112.60
1	A	310	ASP	CA-CB-CG	6.34	118.94	112.60
1	C	563	ASP	CA-CB-CG	6.31	118.91	112.60
1	A	345	ASP	CA-C-N	6.25	132.95	121.70
1	A	345	ASP	C-N-CA	6.25	132.95	121.70
1	B	47	VAL	N-CA-CB	6.17	119.44	111.67
1	A	87	ASP	N-CA-C	-6.13	97.21	107.99
1	A	15	TYR	N-CA-C	-6.09	104.72	111.36
1	B	227	ALA	N-CA-C	-6.08	99.75	109.96
1	A	563	ASP	CA-CB-CG	6.03	118.63	112.60
1	B	106	THR	N-CA-CB	-5.96	101.70	111.66
1	C	49	ALA	N-CA-C	-5.95	104.92	111.82
1	A	343	THR	CA-C-N	5.90	132.31	121.70
1	A	343	THR	C-N-CA	5.90	132.31	121.70
1	A	106	THR	N-CA-CB	-5.82	101.94	111.66
1	C	350	ASN	N-CA-C	-5.79	102.35	109.65
1	B	49	ALA	N-CA-C	-5.62	105.30	111.82
1	C	230	ASP	CA-CB-CG	5.61	118.21	112.60
1	C	22	GLU	CA-C-N	5.58	127.69	120.44
1	C	22	GLU	C-N-CA	5.58	127.69	120.44
1	A	96	ARG	CB-CG-CD	5.43	123.80	111.30
1	B	230	ASP	CA-CB-CG	5.41	118.01	112.60
1	B	345	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	49	ALA	N-CA-C	-5.36	105.60	111.82
1	C	96	ARG	CB-CG-CD	5.24	123.36	111.30
1	B	346	SER	N-CA-C	5.20	116.95	111.28
1	B	378	ASN	CA-C-O	-5.18	115.53	121.54
1	A	578	PRO	CA-C-N	5.17	128.57	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	578	PRO	C-N-CA	5.17	128.57	120.82
1	C	350	ASN	CA-CB-CG	5.16	117.76	112.60
1	B	345	ASP	CA-C-N	5.15	127.18	120.28
1	B	345	ASP	C-N-CA	5.15	127.18	120.28
1	C	441	ASP	N-CA-C	-5.08	103.34	110.35
1	C	348	THR	N-CA-C	5.06	121.57	110.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	451	ILE	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	ARG	Sidechain

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	5025	0	4697	36	0
1	B	5167	0	4930	49	0
1	C	5132	0	4911	42	0
2	A	1	0	0	0	0
3	A	405	0	0	2	0
3	B	565	0	0	2	0
3	C	476	0	0	1	0
All	All	16771	0	14538	111	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 4.

All (111) 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:C:178:MET:HE3	1:C:192:LEU:HD11	1.28	1.12
1:A:178:MET:HE3	1:A:192:LEU:HD11	1.34	1.10
1:B:228:VAL:HG21	1:B:253:MET:HE1	1.43	1.00
1:B:110:ARG:CG	1:B:110:ARG:HH11	1.76	0.99
1:B:110:ARG:HH11	1:B:110:ARG:HG3	1.25	0.98
1:B:156:LEU:CD1	1:B:164:MET:HE1	2.00	0.92
1:B:106:THR:HG21	3:B:813:HOH:O	1.76	0.85
1:A:345:ASP:HA	1:A:346:SER:O	1.76	0.85
1:B:156:LEU:HD12	1:B:164:MET:HE1	1.59	0.84
1:B:106:THR:HG22	1:B:109:ASP:H	1.47	0.78
1:A:106:THR:HG22	1:A:109:ASP:H	1.49	0.77
1:B:110:ARG:HG3	1:B:110:ARG:NH1	2.00	0.77
1:A:106:THR:HG21	3:A:814:HOH:O	1.85	0.76
1:C:178:MET:CE	1:C:192:LEU:HD11	2.12	0.75
1:A:178:MET:CE	1:A:192:LEU:HD11	2.18	0.73
1:B:228:VAL:HG21	1:B:253:MET:CE	2.20	0.72
1:A:96:ARG:HD2	1:C:91:GLU:OE2	1.90	0.71
1:C:346:SER:O	1:C:347:ASN:HB2	1.92	0.70
1:B:249:TYR:HA	1:B:253:MET:HE2	1.72	0.70
1:B:342:TYR:CE2	1:B:387:GLU:HB3	2.29	0.68
1:B:497:GLY:HA3	1:B:502:ALA:O	1.93	0.67
1:B:98:ASP:HA	1:B:110:ARG:HE	1.61	0.66
1:B:238:VAL:HG21	1:B:253:MET:HE3	1.80	0.63
1:A:301:SER:HB3	1:A:304:ASP:HB2	1.80	0.62
1:A:324:SER:H	1:A:328:PRO:HA	1.64	0.61
1:A:156:LEU:HB3	1:A:178:MET:CE	2.31	0.61
1:B:110:ARG:CG	1:B:110:ARG:NH1	2.48	0.61
1:A:214:ALA:HB3	1:A:225:TYR:HB2	1.83	0.61
1:B:91:GLU:OE1	1:C:96:ARG:HD2	2.01	0.59
1:C:27:LEU:HD12	1:C:31:MET:HE3	1.83	0.59
1:B:156:LEU:HD13	1:B:164:MET:HE1	1.82	0.59
1:B:5:LEU:HD12	1:B:27:LEU:HD23	1.85	0.59
1:C:156:LEU:HB3	1:C:178:MET:CE	2.33	0.59
1:A:77:PHE:CE1	1:B:80:MET:HE2	2.37	0.59
1:B:214:ALA:HB3	1:B:225:TYR:HB2	1.85	0.59
1:C:408:ILE:HG22	1:C:409:GLY:H	1.68	0.58
1:A:122:THR:HG21	1:C:122:THR:HG22	1.84	0.58
1:C:214:ALA:HB3	1:C:225:TYR:HB2	1.84	0.57
1:B:293:SER:HB2	1:B:318:ILE:O	2.04	0.57
1:B:96:ARG:C	1:B:110:ARG:HD3	2.30	0.57
1:C:607:ASN:OD1	1:C:612:HIS:HD2	1.89	0.56
1:A:238:VAL:CG1	1:A:253:MET:HB2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:VAL:HG23	1:A:318:ILE:HD11	1.88	0.56
1:B:138:ALA:O	1:B:142:ARG:HB2	2.06	0.55
1:C:207:GLY:HA2	1:C:228:VAL:HG22	1.89	0.54
3:A:1021:HOH:O	1:C:415:HIS:HB3	2.09	0.53
1:B:164:MET:HE2	1:B:178:MET:HB2	1.90	0.52
1:C:138:ALA:O	1:C:142:ARG:HB2	2.09	0.52
1:B:279:PHE:O	1:B:297:VAL:HA	2.10	0.51
1:A:171:PRO:HB2	1:A:395:LEU:HD23	1.91	0.51
1:C:552:THR:HG22	1:C:573:ARG:HG2	1.91	0.51
1:C:93:LYS:HA	1:C:96:ARG:HD3	1.91	0.51
1:C:408:ILE:HG22	1:C:409:GLY:N	2.26	0.51
1:A:138:ALA:O	1:A:142:ARG:HB2	2.10	0.51
1:A:156:LEU:HB3	1:A:178:MET:HE1	1.93	0.51
1:B:289:GLN:H	1:B:292:ASN:ND2	2.09	0.51
1:B:329:MET:HG3	1:B:341:TRP:CZ2	2.46	0.50
1:A:93:LYS:HA	1:A:96:ARG:HD3	1.94	0.50
1:C:612:HIS:HE1	3:C:1112:HOH:O	1.94	0.49
1:B:98:ASP:HA	1:B:110:ARG:NE	2.26	0.49
1:B:280:ARG:HE	1:B:295:ASN:HD21	1.60	0.49
1:A:157:SER:HB3	1:B:445:ARG:HB2	1.95	0.49
1:A:238:VAL:HG12	1:A:253:MET:HB2	1.94	0.49
1:A:345:ASP:HA	1:A:346:SER:C	2.38	0.48
1:C:303:ASP:OD1	1:C:307:LYS:HE3	2.12	0.48
1:A:329:MET:HG3	1:A:341:TRP:CZ2	2.48	0.48
1:B:297:VAL:HG23	1:B:318:ILE:HD11	1.96	0.48
1:A:77:PHE:HZ	1:B:77:PHE:CD2	2.31	0.48
1:A:156:LEU:HD13	1:A:178:MET:HE2	1.96	0.48
1:C:414:ARG:HG2	1:C:414:ARG:HH21	1.78	0.48
1:B:77:PHE:HE1	1:C:77:PHE:HA	1.79	0.47
1:B:316:MET:HG3	1:B:362:LYS:HG2	1.96	0.47
1:B:110:ARG:HH11	1:B:110:ARG:HG2	1.72	0.47
1:C:156:LEU:HB3	1:C:178:MET:HE1	1.97	0.47
1:A:77:PHE:HE1	1:B:80:MET:HE2	1.80	0.46
1:B:29:SER:HB2	1:C:5:LEU:HD12	1.98	0.46
1:C:156:LEU:HD13	1:C:178:MET:HE2	1.96	0.46
1:C:316:MET:HG3	1:C:362:LYS:HG2	1.97	0.45
1:A:328:PRO:HD2	1:A:345:ASP:N	2.31	0.45
1:A:497:GLY:HA3	1:A:502:ALA:O	2.16	0.45
1:A:228:VAL:HG11	1:A:253:MET:HE1	1.98	0.45
1:C:6:ILE:HD12	1:C:20:GLU:HB2	1.99	0.45
1:B:88:GLY:HA2	1:C:85:ASN:ND2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:PHE:O	1:C:297:VAL:HA	2.17	0.44
1:C:346:SER:O	1:C:347:ASN:CB	2.64	0.44
1:A:257:MET:HE3	1:A:305:ILE:O	2.18	0.44
1:C:329:MET:HG3	1:C:341:TRP:CZ2	2.52	0.43
1:B:376:ASN:HD21	1:C:434:ALA:HA	1.83	0.43
1:B:544:TRP:CD1	1:B:544:TRP:H	2.36	0.43
1:C:118:LEU:O	1:C:122:THR:HG23	2.19	0.43
1:B:342:TYR:CZ	1:B:387:GLU:HG2	2.53	0.43
1:B:450:PRO:HG2	1:B:451:ILE:HD12	2.01	0.43
1:C:450:PRO:HG2	1:C:451:ILE:HD12	2.01	0.42
1:A:132:HIS:HD2	3:B:927:HOH:O	2.03	0.42
1:A:249:TYR:HA	1:A:253:MET:HE2	2.02	0.42
1:C:544:TRP:CD1	1:C:544:TRP:H	2.38	0.42
1:C:6:ILE:CD1	1:C:20:GLU:HB2	2.49	0.42
1:B:157:SER:HB3	1:C:445:ARG:HB2	2.01	0.42
1:A:122:THR:CG2	1:C:122:THR:HG22	2.49	0.41
1:B:280:ARG:HE	1:B:295:ASN:ND2	2.18	0.41
1:A:384:GLN:HB2	1:A:408:ILE:HD12	2.02	0.41
1:C:372:ILE:HG21	1:C:419:TYR:CZ	2.55	0.41
1:B:498:HIS:CE1	1:B:500:ASN:HB2	2.56	0.41
1:A:372:ILE:HG21	1:A:419:TYR:CZ	2.56	0.41
1:B:80:MET:HE1	1:C:80:MET:HE1	2.02	0.41
1:A:499:TYR:CD1	1:A:499:TYR:N	2.89	0.41
1:B:224:ILE:O	1:B:239:ARG:HA	2.21	0.41
1:B:498:HIS:HB3	1:C:467:TYR:CG	2.56	0.41
1:C:347:ASN:HB3	1:C:348:THR:H	1.23	0.41
1:A:544:TRP:CD1	1:A:544:TRP:H	2.38	0.41
1:B:80:MET:HE3	1:C:80:MET:SD	2.61	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	627/648 (97%)	598 (95%)	24 (4%)	5 (1%)	16	16
1	B	633/648 (98%)	609 (96%)	21 (3%)	3 (0%)	24	27
1	C	626/648 (97%)	601 (96%)	21 (3%)	4 (1%)	21	23
All	All	1886/1944 (97%)	1808 (96%)	66 (4%)	12 (1%)	21	23

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	346	SER
1	C	347	ASN
1	C	348	THR
1	A	349	ALA
1	A	411	GLY
1	A	608	PHE
1	C	608	PHE
1	B	290	LEU
1	B	608	PHE
1	C	48	PHE
1	A	48	PHE
1	B	411	GLY

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	522/575 (91%)	500 (96%)	22 (4%)	26	36
1	B	554/575 (96%)	534 (96%)	20 (4%)	31	42
1	C	551/575 (96%)	535 (97%)	16 (3%)	37	51
All	All	1627/1725 (94%)	1569 (96%)	58 (4%)	31	42

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLU

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Mol	Chain	Res	Type
1	A	82	LEU
1	A	106	THR
1	A	110	ARG
1	A	137	ARG
1	A	147	GLU
1	A	229	LEU
1	A	248	THR
1	A	251	ASN
1	A	253	MET
1	A	256	VAL
1	A	259	ASN
1	A	305	ILE
1	A	309	ILE
1	A	320	MET
1	A	346	SER
1	A	384	GLN
1	A	385	GLU
1	A	395	LEU
1	A	412	ASN
1	A	446	VAL
1	A	569	GLU
1	B	14	ASP
1	B	40	GLU
1	B	106	THR
1	B	110	ARG
1	B	137	ARG
1	B	146	LYS
1	B	185	ASN
1	B	219	ASP
1	B	243	ARG
1	B	277	MET
1	B	294	LEU
1	B	327	GLN
1	B	355	GLN
1	B	372	ILE
1	B	396	GLU
1	B	406	VAL
1	B	446	VAL
1	B	544	TRP
1	B	569	GLU
1	B	604	ARG
1	C	11	ARG

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Mol	Chain	Res	Type
1	C	21	ASN
1	C	27	LEU
1	C	93	LYS
1	C	110	ARG
1	C	151	GLU
1	C	228	VAL
1	C	277	MET
1	C	288	ARG
1	C	309	ILE
1	C	347	ASN
1	C	348	THR
1	C	377	ASN
1	C	396	GLU
1	C	414	ARG
1	C	446	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	132	HIS
1	A	197	GLN
1	A	213	ASN
1	A	234	ASN
1	A	315	GLN
1	A	347	ASN
1	A	412	ASN
1	A	428	GLN
1	A	432	ASN
1	A	510	ASN
1	A	572	ASN
1	B	21	ASN
1	B	132	HIS
1	B	161	ASN
1	B	241	GLN
1	B	292	ASN
1	B	295	ASN
1	B	327	GLN
1	B	376	ASN
1	B	413	ASN
1	B	432	ASN
1	B	452	GLN

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Mol	Chain	Res	Type
1	B	453	ASN
1	B	572	ASN
1	C	21	ASN
1	C	85	ASN
1	C	113	HIS
1	C	165	GLN
1	C	213	ASN
1	C	241	GLN
1	C	327	GLN
1	C	376	ASN
1	C	500	ASN
1	C	572	ASN
1	C	612	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is 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	631/648 (97%)	0.37	56 (8%)	15 13	28, 52, 100, 134	0
1	B	635/648 (97%)	-0.14	21 (3%)	49 46	27, 43, 71, 119	0
1	C	630/648 (97%)	-0.02	22 (3%)	47 44	28, 47, 79, 120	0
All	All	1896/1944 (97%)	0.07	99 (5%)	33 29	27, 47, 90, 134	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	375	VAL	4.7
1	A	375	VAL	4.5
1	B	386	ALA	4.4
1	B	77	PHE	4.4
1	A	-1	GLY	3.9
1	A	374	GLY	3.8
1	B	450	PRO	3.7
1	A	383	PHE	3.6
1	A	305	ILE	3.6
1	A	294	LEU	3.5
1	A	256	VAL	3.5
1	A	218	ILE	3.5
1	A	283	TYR	3.5
1	A	387	GLU	3.5
1	B	15	TYR	3.4
1	A	349	ALA	3.4
1	A	412	ASN	3.3
1	C	408	ILE	3.3
1	C	383	PHE	3.3
1	A	292	ASN	3.3
1	C	376	ASN	3.3
1	C	377	ASN	3.3
1	C	3	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	372	ILE	3.2
1	B	499	TYR	3.1
1	B	413	ASN	3.1
1	A	261	PHE	3.1
1	A	15	TYR	3.1
1	A	309	ILE	3.1
1	B	349	ALA	3.1
1	C	407	THR	3.0
1	A	302	ALA	2.9
1	C	4	LYS	2.9
1	C	378	ASN	2.9
1	A	359	ILE	2.9
1	A	320	MET	2.9
1	A	3	ASN	2.9
1	A	1	MET	2.8
1	A	406	VAL	2.8
1	A	415	HIS	2.7
1	A	348	THR	2.7
1	A	407	THR	2.7
1	C	409	GLY	2.7
1	A	324	SER	2.7
1	C	410	PRO	2.7
1	A	291	LYS	2.6
1	C	406	VAL	2.6
1	C	372	ILE	2.6
1	C	349	ALA	2.6
1	A	223	TRP	2.6
1	A	232	ASN	2.6
1	C	60	LEU	2.6
1	A	286	THR	2.5
1	A	395	LEU	2.5
1	A	376	ASN	2.4
1	A	293	SER	2.4
1	C	451	ILE	2.4
1	A	237	PHE	2.4
1	C	411	GLY	2.4
1	A	318	ILE	2.4
1	A	312	VAL	2.3
1	A	408	ILE	2.3
1	A	325	ASP	2.3
1	A	345	ASP	2.3
1	C	373	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	13	PHE	2.3
1	B	384	GLN	2.3
1	C	348	THR	2.3
1	B	378	ASN	2.3
1	A	276	LEU	2.2
1	B	326	THR	2.2
1	A	289	GLN	2.2
1	B	451	ILE	2.2
1	A	184	GLY	2.2
1	C	415	HIS	2.2
1	A	260	ILE	2.2
1	A	238	VAL	2.2
1	A	265	TYR	2.1
1	A	314	TYR	2.1
1	C	61	ASN	2.1
1	C	347	ASN	2.1
1	B	379	PHE	2.1
1	B	497	GLY	2.1
1	A	386	ALA	2.1
1	A	219	ASP	2.1
1	B	372	ILE	2.1
1	B	449	LEU	2.1
1	A	384	GLN	2.1
1	A	319	PRO	2.1
1	A	373	GLY	2.1
1	B	346	SER	2.1
1	A	451	ILE	2.1
1	B	500	ASN	2.1
1	B	375	VAL	2.1
1	A	285	PRO	2.0
1	A	410	PRO	2.0
1	B	410	PRO	2.0
1	A	257	MET	2.0
1	B	453	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	A	701	1/1	1.00	0.03	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.