Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:21 pm BST

PDB ID	:	5O7O
Title	:	The crystal structure of DfoC, the desferrioxamine biosynthetic pathway acetyltransferase/Non-Ribosomal Peptide Synthetase (NRPS)-Independent Siderophore (NIS) from the fire blight disease pathogen Erwinia amylovora
Authors	:	Salomone-Stagni, M.; Bartho, J.D.; Polsinelli, I.; Bellini, D.; Walsh, M.A.; Demitri, N.; Benini, S.
Deposited on	:	2017-06-09
Resolution	:	2.11 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 following versions of software and data (see references ①) were used in the production of this report:

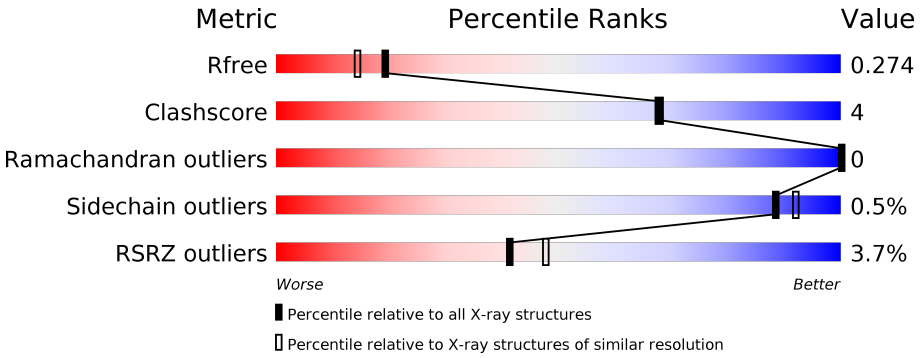
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

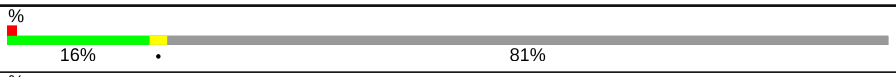
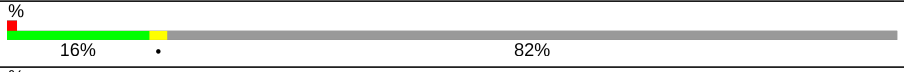
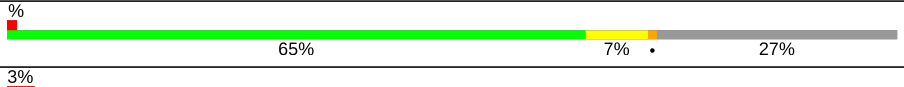
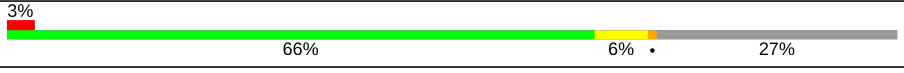
The reported resolution of this entry is 2.11 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	787	
1	B	787	
1	C	787	
1	D	787	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12009 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 Desferrioxamine siderophore biosynthesis protein dfoC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	0	0	0
			1179	754	206	210	9			
1	B	145	Total	C	N	O	S	0	0	0
			1173	752	204	207	10			
1	C	575	Total	C	N	O	S	0	0	0
			4616	2950	803	840	23			
1	D	575	Total	C	N	O	S	0	0	0
			4616	2950	802	841	23			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP D4I247
A	-1	ALA	-	expression tag	UNP D4I247
A	0	MET	-	expression tag	UNP D4I247
A	1	SER	-	expression tag	UNP D4I247
B	-2	GLY	-	expression tag	UNP D4I247
B	-1	ALA	-	expression tag	UNP D4I247
B	0	MET	-	expression tag	UNP D4I247
B	1	SER	-	expression tag	UNP D4I247
C	-2	GLY	-	expression tag	UNP D4I247
C	-1	ALA	-	expression tag	UNP D4I247
C	0	MET	-	expression tag	UNP D4I247
C	1	SER	-	expression tag	UNP D4I247
D	-2	GLY	-	expression tag	UNP D4I247
D	-1	ALA	-	expression tag	UNP D4I247
D	0	MET	-	expression tag	UNP D4I247
D	1	SER	-	expression tag	UNP D4I247

- Molecule 2 is water.

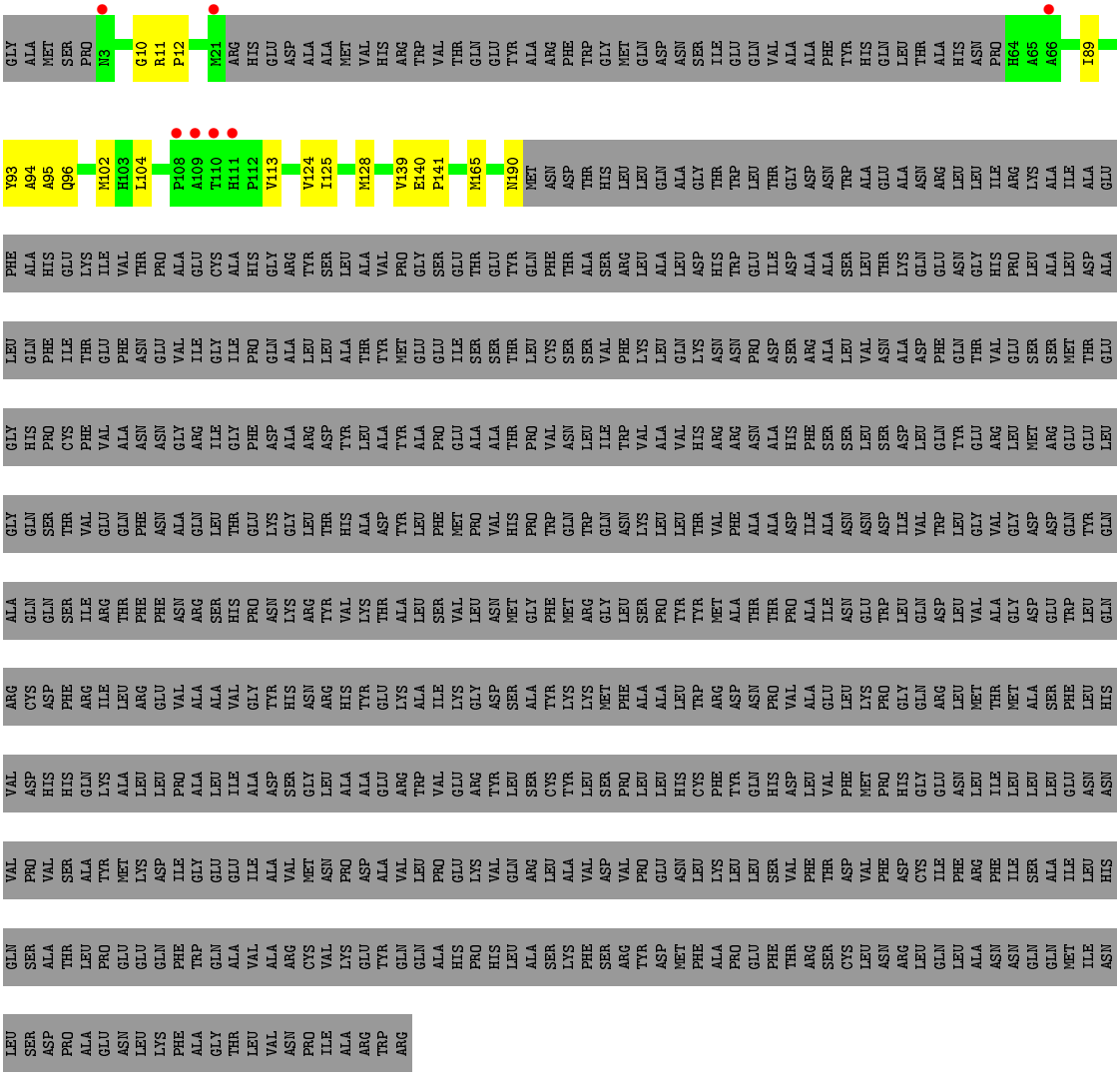
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	30	Total O 30 30	0	0
2	B	32	Total O 32 32	0	0
2	C	195	Total O 195 195	0	0
2	D	168	Total O 168 168	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

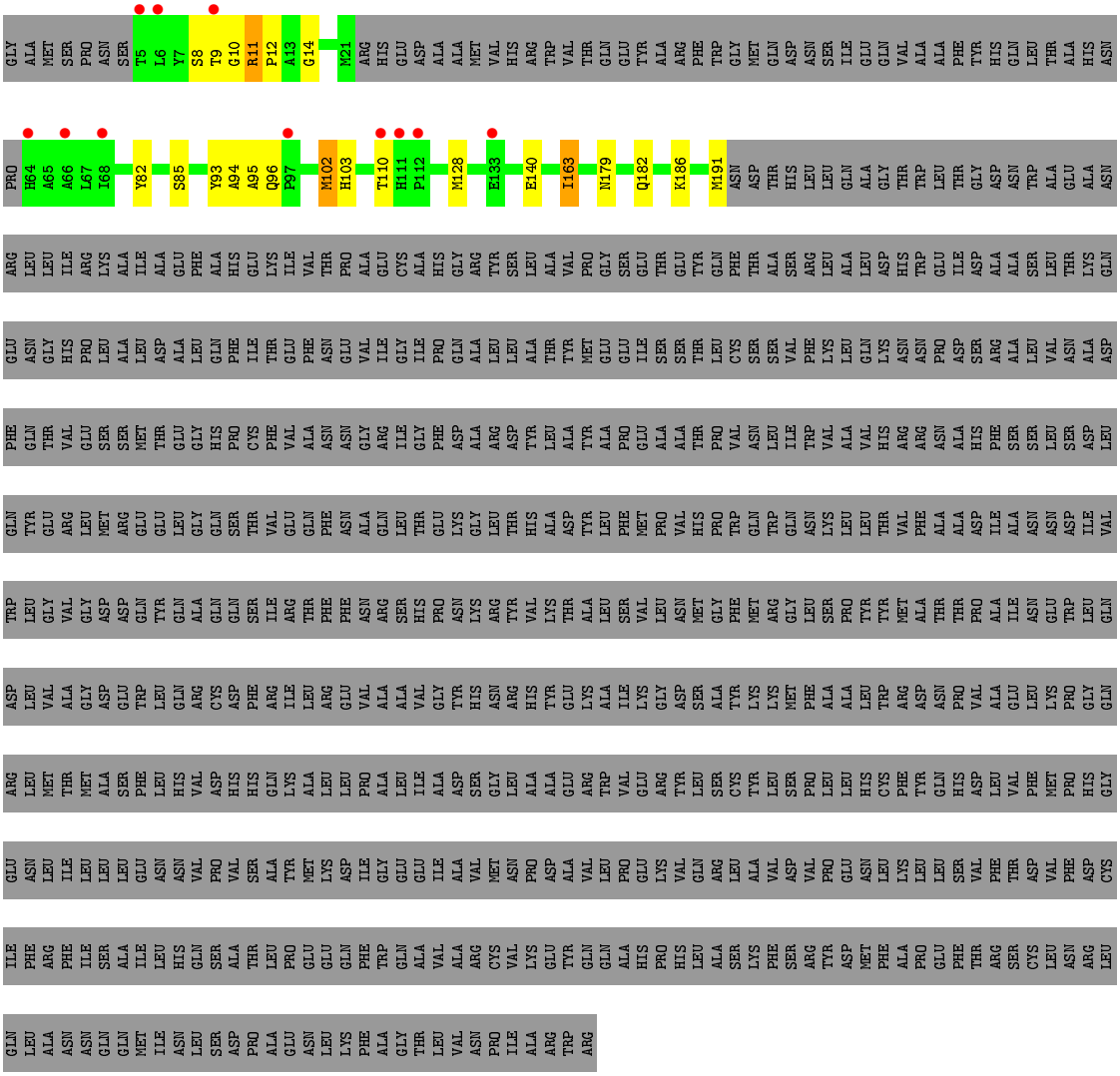
- Molecule 1: Desferrioxamine siderophore biosynthesis protein dfoC

Chain A:



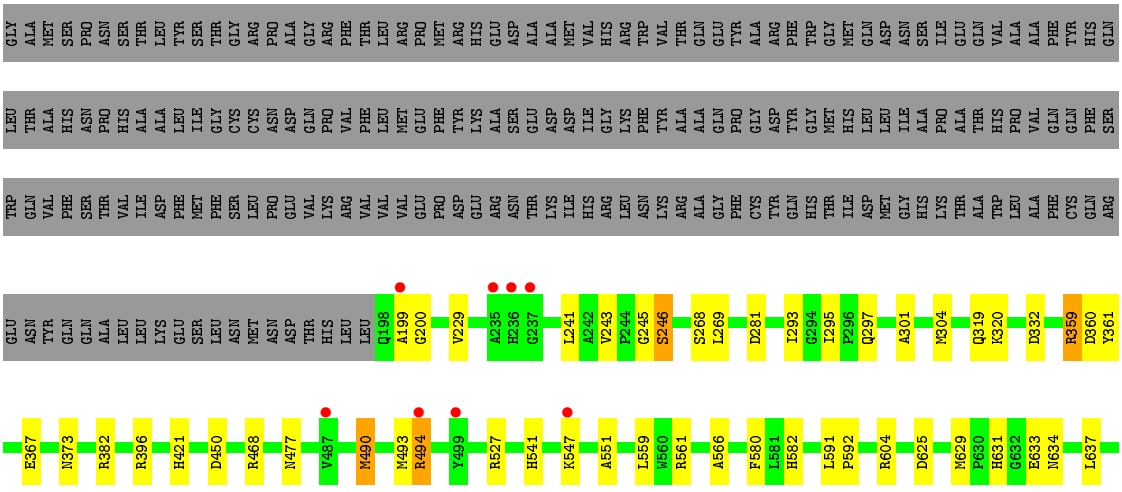
- Molecule 1: Desferrioxamine siderophore biosynthesis protein dfoC

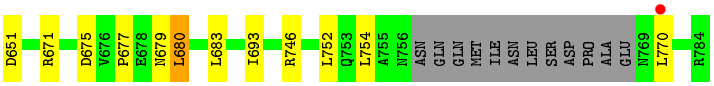
Chain B:



• Molecule 1: Desferrioxamine siderophore biosynthesis protein dfoC

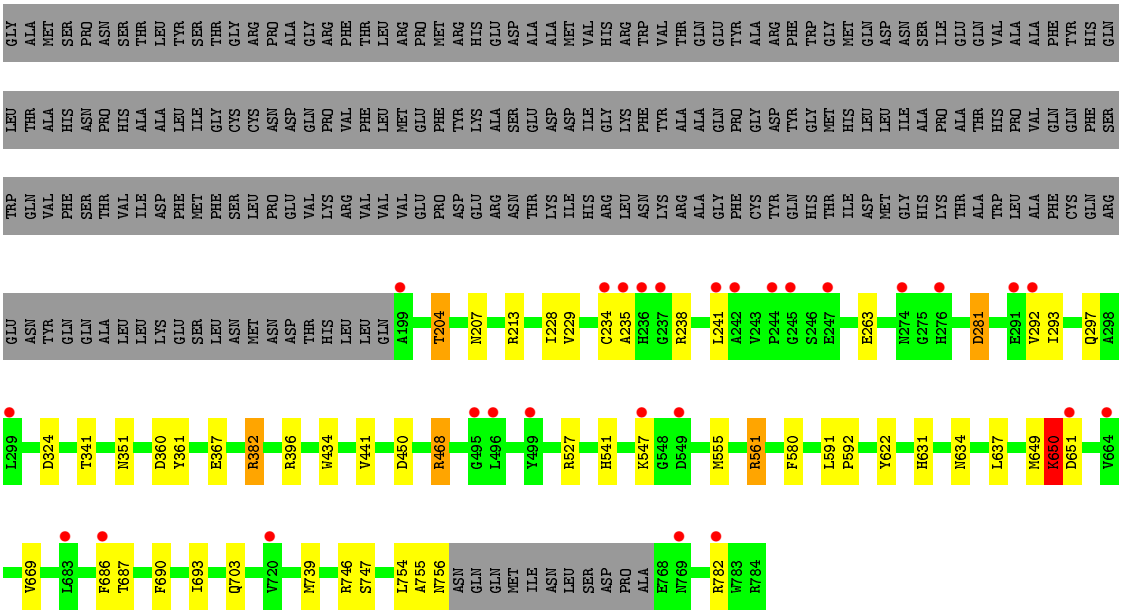
Chain C:





- Molecule 1: Desferrioxamine siderophore biosynthesis protein dfoC

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.17Å 156.35Å 93.81Å 90.00° 95.57° 90.00°	Depositor
Resolution (Å)	78.18 – 2.11 78.17 – 2.11	Depositor EDS
% Data completeness (in resolution range)	99.8 (78.18-2.11) 99.8 (78.17-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.221 , 0.264 0.235 , 0.274	Depositor DCC
R_{free} test set	6119 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	44.9	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 42.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12009	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.94	1/1211 (0.1%)	0.93	4/1638 (0.2%)
1	B	0.90	1/1205 (0.1%)	1.02	8/1629 (0.5%)
1	C	0.87	4/4736 (0.1%)	0.93	19/6440 (0.3%)
1	D	0.83	2/4736 (0.0%)	0.90	14/6440 (0.2%)
All	All	0.86	8/11888 (0.1%)	0.92	45/16147 (0.3%)

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	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	649	MET	C-N	11.38	1.60	1.34
1	C	268	SER	C-N	-11.35	1.07	1.34
1	B	163	ILE	C-N	-11.08	1.08	1.34
1	C	245	GLY	C-N	10.91	1.59	1.34
1	C	246	SER	C-N	-9.44	1.12	1.34
1	C	269	LEU	C-N	-6.63	1.18	1.34
1	D	650	LYS	C-N	-5.87	1.20	1.34
1	A	10	GLY	C-N	-5.12	1.22	1.34

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	490	MET	CB-CA-C	-15.29	79.83	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	163	ILE	O-C-N	-13.47	101.15	122.70
1	B	10	GLY	C-N-CA	10.81	148.73	121.70
1	B	10	GLY	O-C-N	-9.72	107.15	122.70
1	A	10	GLY	C-N-CA	9.54	145.55	121.70
1	A	10	GLY	O-C-N	-9.38	107.69	122.70
1	B	163	ILE	CA-C-N	7.93	134.64	117.20
1	D	561	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	D	746	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	C	527	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	C	746	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	D	281	ASP	CB-CG-OD1	6.94	124.55	118.30
1	B	10	GLY	CA-C-N	6.94	132.46	117.20
1	C	396	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	10	GLY	CA-C-N	6.70	131.94	117.20
1	C	490	MET	N-CA-C	6.62	128.88	111.00
1	C	527	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	D	213	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	C	396	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	D	382	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	D	396	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	D	468	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	C	332	ASP	CB-CG-OD1	6.12	123.80	118.30
1	D	324	ASP	CB-CG-OD1	6.07	123.76	118.30
1	D	396	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	D	782	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	C	561	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	C	359	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	B	11	ARG	O-C-N	5.69	131.91	121.10
1	D	360	ASP	CB-CG-OD1	5.61	123.35	118.30
1	C	268	SER	O-C-N	-5.55	113.82	122.70
1	D	527	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	102	MET	CG-SD-CE	5.49	108.98	100.20
1	C	604	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	D	324	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	A	125	ILE	CG1-CB-CG2	-5.42	99.47	111.40
1	B	163	ILE	C-N-CA	5.39	135.16	121.70
1	C	494	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	D	468	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	C	680	LEU	CA-CB-CG	5.26	127.41	115.30
1	C	671	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	C	625	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	C	360	ASP	CB-CG-OD1	5.14	122.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	268	SER	C-N-CA	5.12	134.51	121.70
1	C	675	ASP	CB-CG-OD1	5.09	122.89	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	163	ILE	Mainchain
1	C	200	GLY	Peptide
1	D	650	LYS	Mainchain

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	1179	0	1142	18	0
1	B	1173	0	1139	14	0
1	C	4616	0	4499	36	0
1	D	4616	0	4499	30	0
2	A	30	0	0	2	0
2	B	32	0	0	0	0
2	C	195	0	0	4	0
2	D	168	0	0	2	0
All	All	12009	0	11279	87	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 (87) 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:A:139:VAL:HG12	1:A:141:PRO:HD3	1.46	0.93
1:D:361:TYR:OH	1:D:367:GLU:OE2	1.91	0.88
1:A:94:ALA:O	1:A:96:GLN:NE2	2.17	0.77
1:A:140:GLU:OE1	1:A:165:MET:CE	2.35	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ILE:HD12	1:A:140:GLU:HB3	1.73	0.69
1:C:293:ILE:HG23	1:C:754:LEU:HD13	1.76	0.68
1:D:235:ALA:HB3	1:D:238:ARG:HB2	1.77	0.67
1:C:229:VAL:CG1	1:C:241:LEU:HD11	2.29	0.62
1:C:680:LEU:HA	1:C:683:LEU:HG	1.82	0.61
1:B:11:ARG:HB3	1:B:12:PRO:HD2	1.82	0.61
1:C:199:ALA:HB1	1:D:434:TRP:HE1	1.65	0.61
1:A:140:GLU:OE1	1:A:165:MET:HE1	2.01	0.60
1:A:11:ARG:HB3	1:A:12:PRO:HD2	1.85	0.58
1:D:229:VAL:CG1	1:D:241:LEU:HD11	2.34	0.58
1:A:140:GLU:O	1:A:140:GLU:HG3	2.03	0.57
1:D:669:VAL:O	1:D:669:VAL:HG12	2.05	0.57
1:D:631:HIS:HA	1:D:693:ILE:HD11	1.86	0.57
1:B:94:ALA:O	1:B:96:GLN:NE2	2.30	0.57
1:D:441:VAL:HG21	1:D:555:MET:HE1	1.88	0.56
1:D:382:ARG:NH1	1:D:450:ASP:OD1	2.38	0.55
1:C:679:ASN:O	1:C:680:LEU:HG	2.06	0.55
1:D:229:VAL:HG13	1:D:241:LEU:HD11	1.88	0.55
1:B:140:GLU:O	1:B:140:GLU:HG2	2.07	0.55
1:A:102:MET:CE	1:A:104:LEU:HB2	2.37	0.54
1:B:186:LYS:HE2	1:C:373:ASN:ND2	2.22	0.54
1:C:382:ARG:NH1	1:C:450:ASP:OD1	2.38	0.53
1:A:113:VAL:HG22	1:B:14:GLY:HA2	1.90	0.53
1:C:541:HIS:HE1	1:D:281:ASP:OD2	1.91	0.53
1:A:102:MET:HE3	1:A:104:LEU:HB2	1.91	0.53
1:C:631:HIS:HA	1:C:693:ILE:HD11	1.91	0.52
1:A:89:ILE:CD1	1:A:140:GLU:HB3	2.37	0.52
1:B:191:MET:CE	1:C:359:ARG:HG2	2.40	0.52
1:D:580:PHE:CE2	1:D:637:LEU:HD13	2.45	0.52
1:C:580:PHE:CE2	1:C:637:LEU:HD13	2.44	0.51
1:D:650:LYS:HE2	2:D:964:HOH:O	2.09	0.51
1:C:320:LYS:O	2:C:801:HOH:O	2.19	0.51
1:C:421:HIS:HD2	2:C:989:HOH:O	1.92	0.51
1:A:140:GLU:OE1	1:A:165:MET:HE3	2.10	0.51
1:D:561:ARG:NH1	1:D:650:LYS:HD2	2.25	0.50
1:D:204:THR:HG22	1:D:207:ASN:HB2	1.94	0.49
1:A:93:TYR:CE2	1:A:95:ALA:HA	2.48	0.49
1:B:102:MET:HG3	1:B:128:MET:HE2	1.95	0.49
1:B:8:SER:O	1:B:9:THR:HG23	2.13	0.48
1:C:281:ASP:OD2	1:D:541:HIS:HE1	1.97	0.48
1:C:295:ILE:N	2:C:808:HOH:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:622:TYR:OH	1:D:739:MET:HG2	2.14	0.48
1:B:191:MET:HE2	1:C:359:ARG:HG2	1.95	0.47
1:C:297:GLN:HE22	1:D:547:LYS:H	1.61	0.47
1:D:634:ASN:OD1	1:D:651:ASP:OD2	2.32	0.47
1:C:582:HIS:HD2	2:C:952:HOH:O	1.98	0.47
1:B:179:ASN:HA	1:B:182:GLN:NE2	2.30	0.47
1:C:301:ALA:HA	1:C:304:MET:HE3	1.97	0.47
1:A:102:MET:HG2	1:A:128:MET:HE2	1.97	0.46
1:D:468:ARG:HD2	2:D:955:HOH:O	2.15	0.46
1:D:234:CYS:SG	1:D:238:ARG:HB3	2.55	0.46
1:C:591:LEU:HB3	1:C:592:PRO:HD3	1.99	0.44
1:D:686:PHE:O	1:D:690:PHE:HB2	2.17	0.44
1:A:190:ASN:HA	2:A:803:HOH:O	2.17	0.44
1:C:361:TYR:OH	1:C:367:GLU:OE2	2.17	0.44
1:D:687:THR:HG21	1:D:747:SER:HB2	1.99	0.44
1:D:228:ILE:O	1:D:292:VAL:CG1	2.65	0.44
1:C:468:ARG:HD3	1:C:494:ARG:HB3	1.99	0.44
1:C:752:LEU:HD21	1:C:770:LEU:HA	2.00	0.44
1:C:547:LYS:H	1:D:297:GLN:HE22	1.65	0.44
1:D:293:ILE:HG23	1:D:754:LEU:HD13	2.00	0.44
1:C:493:MET:HE2	1:C:551:ALA:HB1	2.01	0.43
1:C:547:LYS:N	1:D:297:GLN:HE22	2.16	0.43
1:C:319:GLN:HG2	1:C:319:GLN:O	2.18	0.43
1:C:677:PRO:O	1:C:679:ASN:O	2.37	0.43
1:D:263:GLU:HG2	1:D:703:GLN:HG3	2.00	0.43
1:B:93:TYR:CE2	1:B:95:ALA:HA	2.52	0.43
1:A:11:ARG:HB3	1:A:12:PRO:CD	2.49	0.42
1:B:82:TYR:HE2	1:B:103:HIS:CE1	2.38	0.42
1:A:190:ASN:ND2	2:A:803:HOH:O	2.52	0.41
1:C:243:VAL:O	1:C:246:SER:HB3	2.20	0.41
1:C:629:MET:HG3	1:C:631:HIS:CD2	2.55	0.41
1:C:631:HIS:CE1	1:C:633:GLU:HB3	2.55	0.41
1:A:124:VAL:HG12	1:A:128:MET:HE2	2.02	0.41
1:D:755:ALA:O	1:D:756:ASN:C	2.59	0.41
1:B:82:TYR:CE2	1:B:103:HIS:CE1	3.08	0.41
1:D:591:LEU:HB3	1:D:592:PRO:HD3	2.03	0.41
1:D:687:THR:HG21	1:D:747:SER:CB	2.51	0.40
1:C:559:LEU:HD12	1:C:559:LEU:C	2.41	0.40
1:C:634:ASN:ND2	1:C:651:ASP:OD2	2.54	0.40
1:B:191:MET:CE	1:C:359:ARG:CG	2.98	0.40
1:C:229:VAL:HG13	1:C:241:LEU:HD11	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:ASN:HD22	1:C:566:ALA:HA	1.87	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	142/787 (18%)	136 (96%)	6 (4%)	0	100	100
1	B	141/787 (18%)	136 (96%)	5 (4%)	0	100	100
1	C	571/787 (73%)	551 (96%)	20 (4%)	0	100	100
1	D	571/787 (73%)	552 (97%)	19 (3%)	0	100	100
All	All	1425/3148 (45%)	1375 (96%)	50 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	126/670 (19%)	126 (100%)	0	100	100
1	B	125/670 (19%)	123 (98%)	2 (2%)	62	68
1	C	488/670 (73%)	487 (100%)	1 (0%)	93	96
1	D	488/670 (73%)	485 (99%)	3 (1%)	86	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1227/2680 (46%)	1221 (100%)	6 (0%)	88 92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	85	SER
1	B	110	THR
1	C	490	MET
1	D	204	THR
1	D	341	THR
1	D	351	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	182	GLN
1	C	290	ASN
1	C	297	GLN
1	C	334	GLN
1	C	351	ASN
1	C	373	ASN
1	C	464	GLN
1	C	477	ASN
1	C	489	ASN
1	C	522	GLN
1	C	541	HIS
1	C	582	HIS
1	C	624	HIS
1	C	634	ASN
1	C	703	GLN
1	D	274	ASN
1	D	297	GLN
1	D	411	ASN
1	D	541	HIS
1	D	624	HIS
1	D	631	HIS
1	D	725	GLN

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	3
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	269:LEU	C	270:THR	N	1.18
1	C	246:SER	C	247:GLU	N	1.12
1	B	163:ILE	C	164:ASP	N	1.08
1	C	268:SER	C	269:LEU	N	1.07

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	146/787 (18%)	0.30	7 (4%) 30 35	36, 51, 70, 95	0
1	B	145/787 (18%)	0.40	11 (7%) 13 17	37, 55, 74, 84	0
1	C	575/787 (73%)	0.20	9 (1%) 72 76	34, 49, 73, 104	0
1	D	575/787 (73%)	0.25	27 (4%) 31 36	33, 50, 75, 115	0
All	All	1441/3148 (45%)	0.25	54 (3%) 41 48	33, 50, 74, 115	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	499	TYR	7.8
1	C	494	ARG	5.6
1	D	236	HIS	5.3
1	D	495	GLY	5.1
1	A	110	THR	5.0
1	A	111	HIS	4.8
1	D	242	ALA	4.1
1	D	245	GLY	4.0
1	B	6	LEU	3.9
1	D	241	LEU	3.8
1	D	237	GLY	3.6
1	A	66	ALA	3.4
1	C	499	TYR	3.3
1	D	664	VAL	3.2
1	D	235	ALA	3.1
1	C	547	LYS	3.1
1	C	235	ALA	3.0
1	B	112	PRO	3.0
1	A	109	ALA	3.0
1	D	496	LEU	3.0
1	A	21	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	276	HIS	2.8
1	D	199	ALA	2.8
1	D	291	GLU	2.8
1	D	247	GLU	2.7
1	A	108	PRO	2.7
1	C	236	HIS	2.6
1	B	64	HIS	2.6
1	D	244	PRO	2.6
1	D	299	LEU	2.6
1	D	782	ARG	2.5
1	D	769	ASN	2.5
1	D	292	VAL	2.5
1	C	770	LEU	2.5
1	D	234	CYS	2.5
1	B	97	PRO	2.4
1	B	66	ALA	2.4
1	C	237	GLY	2.4
1	B	111	HIS	2.4
1	B	9	THR	2.2
1	A	3	ASN	2.2
1	D	274	ASN	2.2
1	B	110	THR	2.1
1	D	683	LEU	2.1
1	B	68	ILE	2.1
1	C	487	VAL	2.1
1	D	720	VAL	2.1
1	C	199	ALA	2.1
1	D	651	ASP	2.1
1	D	549	ASP	2.0
1	D	547	LYS	2.0
1	D	686	PHE	2.0
1	B	133	GLU	2.0
1	B	5	THR	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.