



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:26 PM UTC

PDB ID : 5O7O / pdb\_00005o7o  
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](mailto: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>.

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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

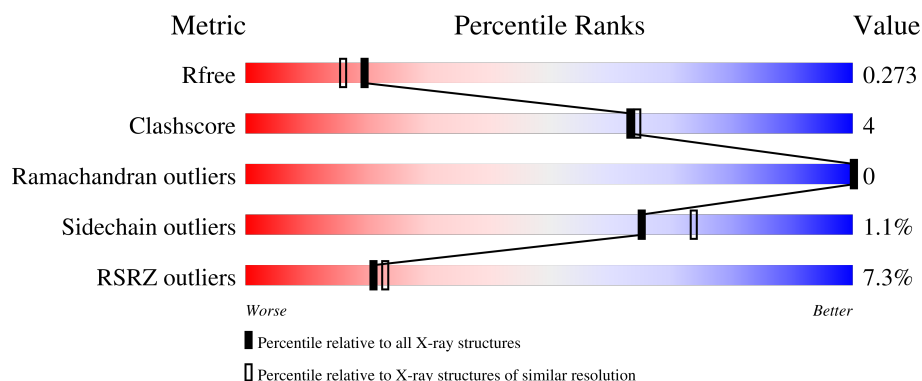
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.11 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))
$R_{free}$	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	787	<div> <div>2%</div> <div>16%</div> <div>81%</div> </div>
1	B	787	<div> <div>3%</div> <div>15%</div> <div>82%</div> </div>
1	C	787	<div> <div>4%</div> <div>65%</div> <div>7%</div> <div>27%</div> </div>
1	D	787	<div> <div>4%</div> <div>66%</div> <div>7%</div> <div>27%</div> </div>

## 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

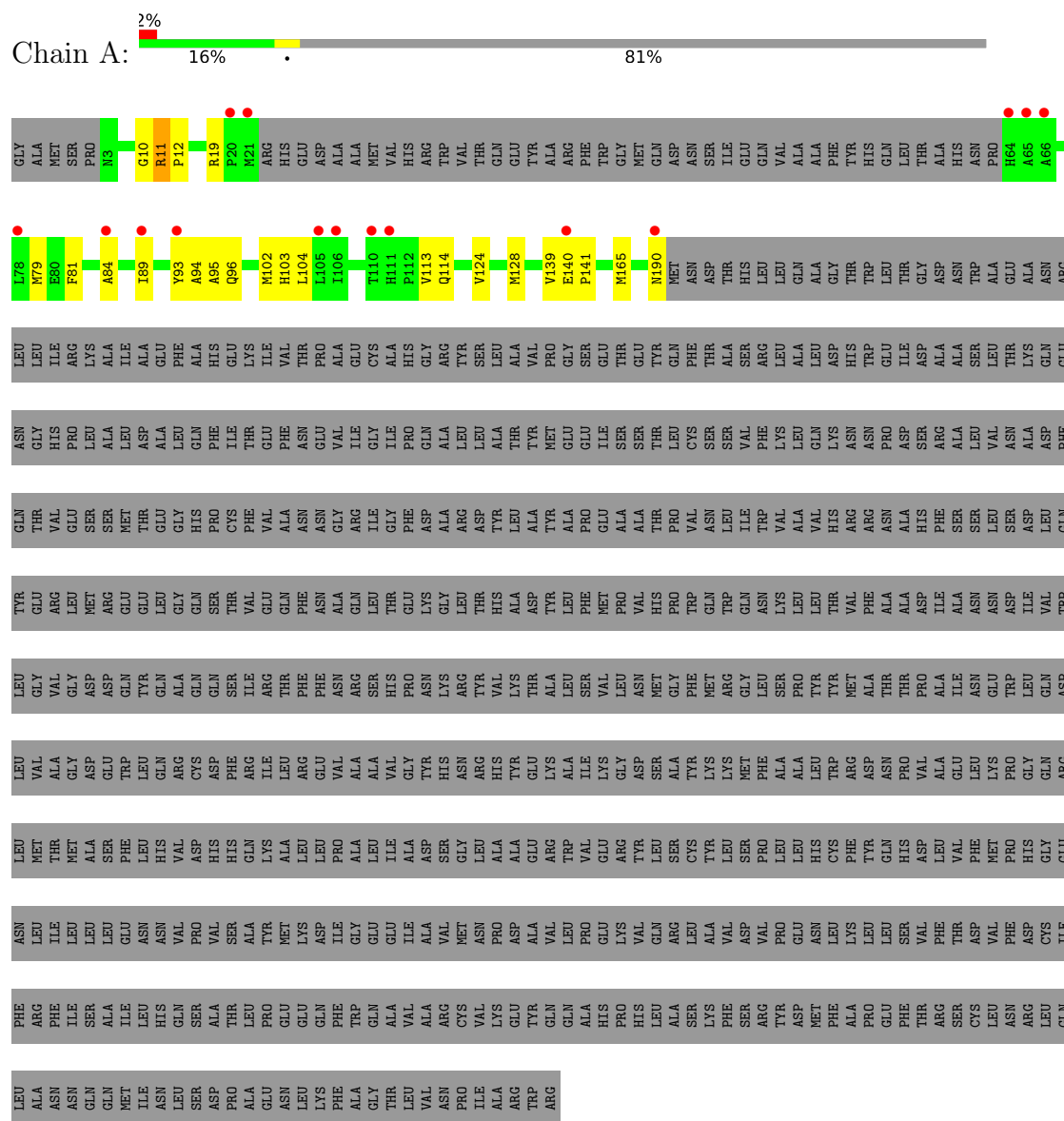
- Molecule 2 is water.

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

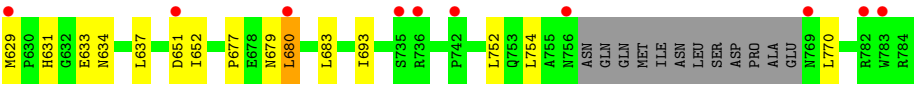
- Molecule 1: Desferrioxamine siderophore biosynthesis protein dfoC



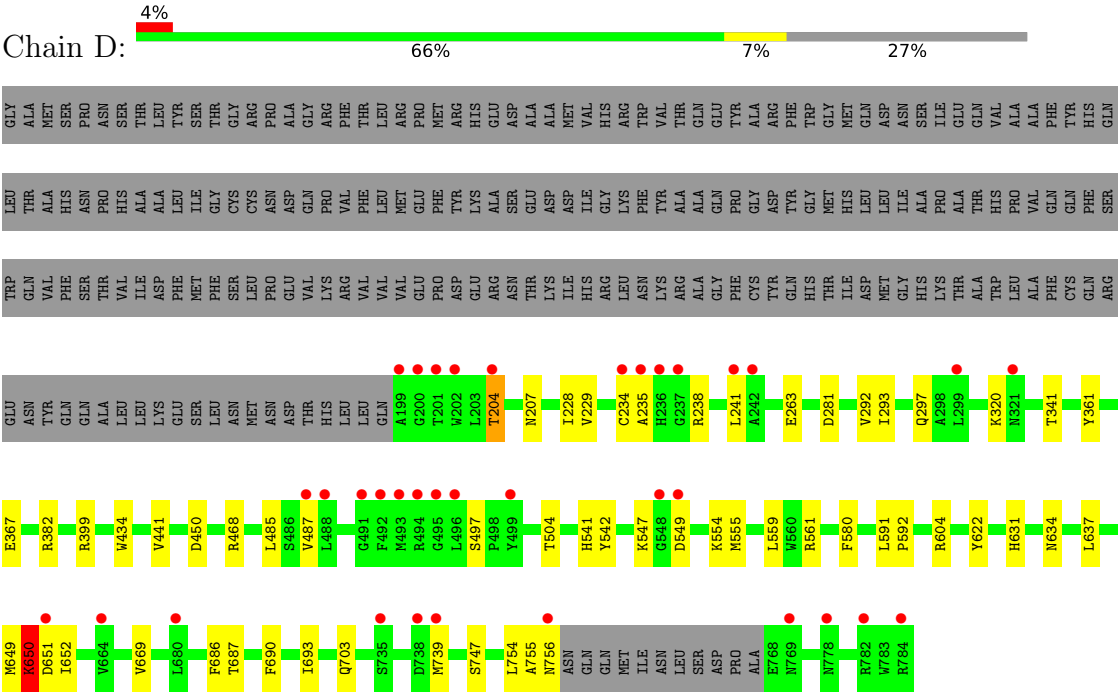
- Molecule 1: Desferrioxamine siderophore biosynthesis protein dfoC







● Molecule 1: Desferrioxamine siderophore biosynthesis protein dfoC



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.17Å 156.35Å 93.81Å 90.00° 95.57° 90.00°	Depositor
Resolution (Å)	78.18 – 2.11 78.18 – 2.11	Depositor EDS
% Data completeness (in resolution range)	99.8 (78.18-2.11) 99.8 (78.18-2.11)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.221 , 0.264 0.235 , 0.273	Depositor DCC
$R_{free}$ test set	6119 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.9	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 28.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 ⓘ

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	1.33	3/1211 (0.2%)	1.33	6/1638 (0.4%)
1	B	1.25	1/1205 (0.1%)	1.40	7/1629 (0.4%)
1	C	1.22	7/4736 (0.1%)	1.11	13/6440 (0.2%)
1	D	1.12	4/4736 (0.1%)	1.04	5/6440 (0.1%)
All	All	1.20	15/11888 (0.1%)	1.14	31/16147 (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	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	245	GLY	C-N	20.95	1.59	1.33
1	D	649	MET	C-N	18.87	1.60	1.33
1	C	268	SER	C-N	-18.11	1.07	1.33
1	B	163	ILE	C-N	-15.14	1.08	1.33
1	C	246	SER	C-N	-14.86	1.12	1.33
1	C	269	LEU	C-N	-10.45	1.18	1.33
1	D	650	LYS	C-N	-9.58	1.20	1.33
1	A	10	GLY	C-N	-8.61	1.22	1.32
1	A	19	ARG	N-CA	6.30	1.50	1.45
1	C	543	GLU	C-O	-6.08	1.16	1.24
1	D	485	LEU	C-O	-5.53	1.17	1.23
1	A	11	ARG	C-O	-5.41	1.19	1.24
1	C	520	TRP	CA-C	5.36	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	456	VAL	C-O	-5.29	1.17	1.24
1	D	399	ARG	C-O	-5.12	1.18	1.24

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	GLY	O-C-N	-20.67	107.69	123.61
1	B	163	ILE	O-C-N	-20.42	101.15	123.00
1	B	10	GLY	CA-C-N	17.20	148.73	123.96
1	B	10	GLY	C-N-CA	17.20	148.73	123.96
1	B	10	GLY	O-C-N	-15.70	107.15	123.48
1	C	490	MET	CB-CA-C	-15.37	79.83	110.42
1	A	10	GLY	CA-C-N	15.00	145.55	123.96
1	A	10	GLY	C-N-CA	15.00	145.55	123.96
1	B	11	ARG	O-C-N	12.46	131.91	121.32
1	D	652	ILE	N-CA-C	12.17	121.97	110.53
1	B	163	ILE	CA-C-N	9.48	135.16	122.84
1	B	163	ILE	C-N-CA	9.48	135.16	122.84
1	C	268	SER	CA-C-N	9.05	134.51	122.30
1	C	268	SER	C-N-CA	9.05	134.51	122.30
1	C	490	MET	N-CA-C	8.49	128.88	110.80
1	C	652	ILE	N-CA-C	7.49	118.42	111.45
1	D	320	LYS	N-CA-C	-7.02	101.07	110.55
1	A	11	ARG	CA-C-N	6.94	126.75	119.05
1	A	11	ARG	C-N-CA	6.94	126.75	119.05
1	C	421	HIS	N-CA-C	5.94	117.76	111.28
1	C	319	GLN	N-CA-C	5.92	118.69	111.82
1	C	268	SER	O-C-N	-5.90	113.82	122.43
1	D	652	ILE	CB-CA-C	-5.89	104.31	112.02
1	C	201	THR	N-CA-C	5.85	117.74	111.36
1	C	680	LEU	N-CA-C	5.73	123.01	110.80
1	A	84	ALA	N-CA-C	5.60	117.38	111.28
1	C	652	ILE	CB-CA-C	-5.47	104.75	111.92
1	C	435	GLN	N-CA-C	5.17	116.99	111.36
1	D	487	VAL	CB-CA-C	-5.12	103.15	110.12
1	C	494	ARG	N-CA-C	5.03	118.31	112.97
1	D	497	SER	N-CA-C	5.02	116.66	109.04

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	19	0
1	B	1173	0	1140	15	0
1	C	4616	0	4500	37	0
1	D	4616	0	4500	33	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	11282	92	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 (92) 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:140:GLU:OE1	1:A:165:MET:HE1	1.45	1.13
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	0.70
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:361:TYR:OH	1:C:367:GLU:OE2	2.17	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:441:VAL:HG21	1:D:555:MET:HE1	1.85	0.58
1:A:140:GLU:O	1:A:140:GLU:HG3	2.03	0.57
1:D:631:HIS:HA	1:D:693:ILE:HD11	1.86	0.57
1:D:669:VAL:HG12	1:D:669:VAL:O	2.05	0.57
1:B:94:ALA:O	1:B:96:GLN:NE2	2.30	0.57
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:HG2	1:B:140:GLU:O	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:79:MET:HE2	1:A:81:PHE:HB2	1.89	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:A:102:MET:HE2	1:A:103:HIS:C	2.35	0.51
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:D:549:ASP:CG	1:D:554:LYS:HZ3	2.19	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:A:124:VAL:HG12	1:A:128:MET:HE2	1.94	0.48
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
1:D:622:TYR:OH	1:D:739:MET:HG2	2.14	0.48
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:79:MET:HE2	1:B:81:PHE:HB2	1.96	0.47
1:B:179:ASN:HA	1:B:182:GLN:NE2	2.30	0.47
1:D:468:ARG:HD2	2:D:955:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:MET:HE1	1:C:359:ARG:HG2	1.98	0.46
1:D:755:ALA:O	1:D:756:ASN:C	2.59	0.46
1:C:486:SER:HB3	1:C:493:MET:HE1	1.98	0.46
1:D:234:CYS:SG	1:D:238:ARG:HB3	2.55	0.46
1:C:559:LEU:HD12	1:C:559:LEU:C	2.41	0.45
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: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:547:LYS:N	1:D:297:GLN:HE22	2.16	0.43
1:C:319:GLN:O	1:C:319:GLN:HG2	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:102:MET:HE1	1:A:104:LEU:HB2	2.01	0.43
1:A:113:VAL:O	1:A:114:GLN:C	2.61	0.42
1:C:304:MET:HE3	1:D:542:TYR:CE2	2.54	0.42
1:D:559:LEU:C	1:D:559:LEU:HD12	2.45	0.42
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:C:427:MET:HE3	1:C:558:ALA:HB2	2.02	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:B:125:ILE:HD13	1:B:128:MET:HE3	2.02	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: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
1:C:477:ASN:HD22	1:C:566:ALA:HA	1.87	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	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

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%)	122 (98%)	3 (2%)	43	48
1	C	488/670 (73%)	482 (99%)	6 (1%)	63	71
1	D	488/670 (73%)	484 (99%)	4 (1%)	73	80
All	All	1227/2680 (46%)	1214 (99%)	13 (1%)	65	74

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	76	VAL
1	B	110	THR

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Mol	Chain	Res	Type
1	B	138	VAL
1	C	201	THR
1	C	427	MET
1	C	490	MET
1	C	504	THR
1	C	546	ILE
1	C	604	ARG
1	D	204	THR
1	D	341	THR
1	D	504	THR
1	D	604	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	ASN
1	B	182	GLN
1	C	274	ASN
1	C	276	HIS
1	C	290	ASN
1	C	297	GLN
1	C	334	GLN
1	C	351	ASN
1	C	373	ASN
1	C	448	ASN
1	C	464	GLN
1	C	477	ASN
1	C	522	GLN
1	C	541	HIS
1	C	624	HIS
1	C	634	ASN
1	C	703	GLN
1	C	711	GLN
1	D	274	ASN
1	D	297	GLN
1	D	411	ASN
1	D	421	HIS
1	D	448	ASN
1	D	465	GLN
1	D	512	GLN
1	D	522	GLN
1	D	541	HIS

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Mol	Chain	Res	Type
1	D	624	HIS
1	D	631	HIS
1	D	725	GLN

### 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](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	146/787 (18%)	0.81	15 (10%)	12 13	36, 51, 70, 95	0
1	B	145/787 (18%)	0.89	24 (16%)	4 5	37, 55, 74, 84	0
1	C	575/787 (73%)	0.53	31 (5%)	31 34	34, 49, 73, 104	0
1	D	575/787 (73%)	0.52	35 (6%)	27 29	33, 50, 75, 115	0
All	All	1441/3148 (45%)	0.59	105 (7%)	21 23	33, 50, 74, 115	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	488	LEU	8.2
1	D	495	GLY	6.4
1	D	199	ALA	6.1
1	A	110	THR	5.8
1	C	492	PHE	5.8
1	A	66	ALA	5.3
1	C	494	ARG	5.3
1	D	299	LEU	5.0
1	A	21	MET	5.0
1	C	199	ALA	4.8
1	C	491	GLY	4.5
1	C	237	GLY	4.5
1	D	651	ASP	4.2
1	D	235	ALA	4.2
1	C	680	LEU	4.1
1	D	499	TYR	4.0
1	B	66	ALA	3.8
1	D	496	LEU	3.6
1	C	200	GLY	3.6
1	C	756	ASN	3.6
1	A	64	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	499	TYR	3.5
1	C	489	ASN	3.4
1	C	487	VAL	3.3
1	D	488	LEU	3.3
1	D	234	CYS	3.3
1	C	735	SER	3.3
1	A	111	HIS	3.2
1	D	735	SER	3.2
1	C	236	HIS	3.1
1	D	242	ALA	3.0
1	B	191	MET	3.0
1	C	493	MET	3.0
1	A	65	ALA	3.0
1	D	492	PHE	3.0
1	C	235	ALA	2.9
1	A	84	ALA	2.9
1	C	490	MET	2.9
1	B	64	HIS	2.9
1	D	237	GLY	2.8
1	B	97	PRO	2.8
1	D	321	ASN	2.8
1	B	89	ILE	2.8
1	C	198	GLN	2.7
1	C	495	GLY	2.7
1	B	6	LEU	2.7
1	D	680	LEU	2.7
1	B	112	PRO	2.7
1	D	549	ASP	2.7
1	B	65	ALA	2.7
1	B	78	LEU	2.7
1	C	500	TYR	2.7
1	D	201	THR	2.6
1	D	236	HIS	2.6
1	B	68	ILE	2.6
1	B	109	ALA	2.6
1	A	93	TYR	2.6
1	D	204	THR	2.6
1	B	21	MET	2.5
1	D	738	ASP	2.5
1	B	140	GLU	2.5
1	C	292	VAL	2.5
1	C	291	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	782	ARG	2.5
1	D	784	ARG	2.5
1	B	76	VAL	2.4
1	D	493	MET	2.4
1	D	202	TRP	2.4
1	D	778	ASN	2.4
1	C	651	ASP	2.4
1	A	89	ILE	2.4
1	C	782	ARG	2.4
1	B	5	THR	2.4
1	A	106	ILE	2.3
1	B	110	THR	2.3
1	A	20	PRO	2.3
1	C	547	LYS	2.3
1	D	548	GLY	2.3
1	D	494	ARG	2.2
1	B	94	ALA	2.2
1	D	739	MET	2.2
1	B	18	LEU	2.2
1	B	105	LEU	2.2
1	D	241	LEU	2.2
1	A	190	ASN	2.2
1	C	783	TRP	2.2
1	B	20	PRO	2.1
1	A	140	GLU	2.1
1	C	629	MET	2.1
1	C	742	PRO	2.1
1	C	202	TRP	2.1
1	D	200	GLY	2.1
1	D	491	GLY	2.1
1	D	487	VAL	2.1
1	B	92	PHE	2.1
1	A	78	LEU	2.0
1	C	769	ASN	2.0
1	D	769	ASN	2.0
1	B	103	HIS	2.0
1	B	82	TYR	2.0
1	B	163	ILE	2.0
1	D	664	VAL	2.0
1	D	756	ASN	2.0
1	A	105	LEU	2.0
1	C	736	ARG	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.