Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:33 PM GMT

PDB ID	:	4FC4
Title	:	FNT family ion channel
Authors	:	Lue , W.; Schwarzer, N.; Du, J.; Gerbig-Smentek, E.; Andrade, S.L.A.; Einsle, O.
Deposited on	:	2012-05-24
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

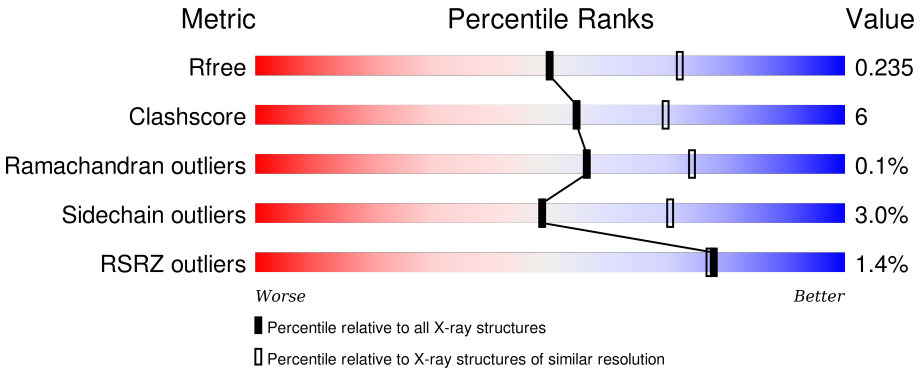
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	261	2% 79% 15% • 5%
1	B	261	2% 79% 15% • •
1	C	261	77% 18% • •
1	D	261	2% 76% 18% • 5%
1	E	261	79% 14% • •

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Mol	Chain	Length	Quality of chain
1	F	261	2% 71% 22%
1	G	261	4% 81% 13% 5%
1	H	261	79% 15%
1	I	261	2% 84% 11%
1	J	261	81% 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BOG	F	302	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19016 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 Nitrite transporter NirC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1874	1241	303	318	12			
1	B	250	Total	C	N	O	S	0	0	0
			1881	1246	304	319	12			
1	C	250	Total	C	N	O	S	0	0	0
			1881	1246	304	319	12			
1	D	249	Total	C	N	O	S	0	0	0
			1873	1241	303	318	11			
1	E	250	Total	C	N	O	S	0	0	0
			1881	1246	304	319	12			
1	F	250	Total	C	N	O	S	0	0	0
			1881	1246	304	319	12			
1	G	248	Total	C	N	O	S	0	0	0
			1866	1236	302	317	11			
1	H	250	Total	C	N	O	S	0	0	0
			1881	1246	304	319	12			
1	I	250	Total	C	N	O	S	0	0	0
			1881	1246	304	319	12			
1	J	250	Total	C	N	O	S	0	0	0
			1881	1246	304	319	12			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	LEU	-	EXPRESSION TAG	UNP E8XEH9
A	255	GLU	-	EXPRESSION TAG	UNP E8XEH9
A	256	HIS	-	EXPRESSION TAG	UNP E8XEH9
A	257	HIS	-	EXPRESSION TAG	UNP E8XEH9
A	258	HIS	-	EXPRESSION TAG	UNP E8XEH9
A	259	HIS	-	EXPRESSION TAG	UNP E8XEH9
A	260	HIS	-	EXPRESSION TAG	UNP E8XEH9
A	261	HIS	-	EXPRESSION TAG	UNP E8XEH9
B	254	LEU	-	EXPRESSION TAG	UNP E8XEH9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	255	GLU	-	EXPRESSION TAG	UNP E8XEH9
B	256	HIS	-	EXPRESSION TAG	UNP E8XEH9
B	257	HIS	-	EXPRESSION TAG	UNP E8XEH9
B	258	HIS	-	EXPRESSION TAG	UNP E8XEH9
B	259	HIS	-	EXPRESSION TAG	UNP E8XEH9
B	260	HIS	-	EXPRESSION TAG	UNP E8XEH9
B	261	HIS	-	EXPRESSION TAG	UNP E8XEH9
C	254	LEU	-	EXPRESSION TAG	UNP E8XEH9
C	255	GLU	-	EXPRESSION TAG	UNP E8XEH9
C	256	HIS	-	EXPRESSION TAG	UNP E8XEH9
C	257	HIS	-	EXPRESSION TAG	UNP E8XEH9
C	258	HIS	-	EXPRESSION TAG	UNP E8XEH9
C	259	HIS	-	EXPRESSION TAG	UNP E8XEH9
C	260	HIS	-	EXPRESSION TAG	UNP E8XEH9
C	261	HIS	-	EXPRESSION TAG	UNP E8XEH9
D	254	LEU	-	EXPRESSION TAG	UNP E8XEH9
D	255	GLU	-	EXPRESSION TAG	UNP E8XEH9
D	256	HIS	-	EXPRESSION TAG	UNP E8XEH9
D	257	HIS	-	EXPRESSION TAG	UNP E8XEH9
D	258	HIS	-	EXPRESSION TAG	UNP E8XEH9
D	259	HIS	-	EXPRESSION TAG	UNP E8XEH9
D	260	HIS	-	EXPRESSION TAG	UNP E8XEH9
D	261	HIS	-	EXPRESSION TAG	UNP E8XEH9
E	254	LEU	-	EXPRESSION TAG	UNP E8XEH9
E	255	GLU	-	EXPRESSION TAG	UNP E8XEH9
E	256	HIS	-	EXPRESSION TAG	UNP E8XEH9
E	257	HIS	-	EXPRESSION TAG	UNP E8XEH9
E	258	HIS	-	EXPRESSION TAG	UNP E8XEH9
E	259	HIS	-	EXPRESSION TAG	UNP E8XEH9
E	260	HIS	-	EXPRESSION TAG	UNP E8XEH9
E	261	HIS	-	EXPRESSION TAG	UNP E8XEH9
F	254	LEU	-	EXPRESSION TAG	UNP E8XEH9
F	255	GLU	-	EXPRESSION TAG	UNP E8XEH9
F	256	HIS	-	EXPRESSION TAG	UNP E8XEH9
F	257	HIS	-	EXPRESSION TAG	UNP E8XEH9
F	258	HIS	-	EXPRESSION TAG	UNP E8XEH9
F	259	HIS	-	EXPRESSION TAG	UNP E8XEH9
F	260	HIS	-	EXPRESSION TAG	UNP E8XEH9
F	261	HIS	-	EXPRESSION TAG	UNP E8XEH9
G	254	LEU	-	EXPRESSION TAG	UNP E8XEH9
G	255	GLU	-	EXPRESSION TAG	UNP E8XEH9
G	256	HIS	-	EXPRESSION TAG	UNP E8XEH9

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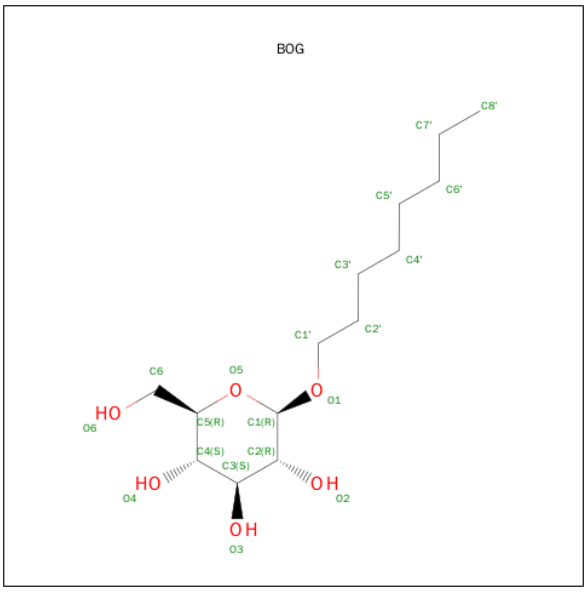
Chain	Residue	Modelled	Actual	Comment	Reference
G	257	HIS	-	EXPRESSION TAG	UNP E8XEH9
G	258	HIS	-	EXPRESSION TAG	UNP E8XEH9
G	259	HIS	-	EXPRESSION TAG	UNP E8XEH9
G	260	HIS	-	EXPRESSION TAG	UNP E8XEH9
G	261	HIS	-	EXPRESSION TAG	UNP E8XEH9
H	254	LEU	-	EXPRESSION TAG	UNP E8XEH9
H	255	GLU	-	EXPRESSION TAG	UNP E8XEH9
H	256	HIS	-	EXPRESSION TAG	UNP E8XEH9
H	257	HIS	-	EXPRESSION TAG	UNP E8XEH9
H	258	HIS	-	EXPRESSION TAG	UNP E8XEH9
H	259	HIS	-	EXPRESSION TAG	UNP E8XEH9
H	260	HIS	-	EXPRESSION TAG	UNP E8XEH9
H	261	HIS	-	EXPRESSION TAG	UNP E8XEH9
I	254	LEU	-	EXPRESSION TAG	UNP E8XEH9
I	255	GLU	-	EXPRESSION TAG	UNP E8XEH9
I	256	HIS	-	EXPRESSION TAG	UNP E8XEH9
I	257	HIS	-	EXPRESSION TAG	UNP E8XEH9
I	258	HIS	-	EXPRESSION TAG	UNP E8XEH9
I	259	HIS	-	EXPRESSION TAG	UNP E8XEH9
I	260	HIS	-	EXPRESSION TAG	UNP E8XEH9
I	261	HIS	-	EXPRESSION TAG	UNP E8XEH9
J	254	LEU	-	EXPRESSION TAG	UNP E8XEH9
J	255	GLU	-	EXPRESSION TAG	UNP E8XEH9
J	256	HIS	-	EXPRESSION TAG	UNP E8XEH9
J	257	HIS	-	EXPRESSION TAG	UNP E8XEH9
J	258	HIS	-	EXPRESSION TAG	UNP E8XEH9
J	259	HIS	-	EXPRESSION TAG	UNP E8XEH9
J	260	HIS	-	EXPRESSION TAG	UNP E8XEH9
J	261	HIS	-	EXPRESSION TAG	UNP E8XEH9

- Molecule 2 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total C O 20 14 6	0	0
2	F	1	Total C O 20 14 6	0	0

- Molecule 3 is water.

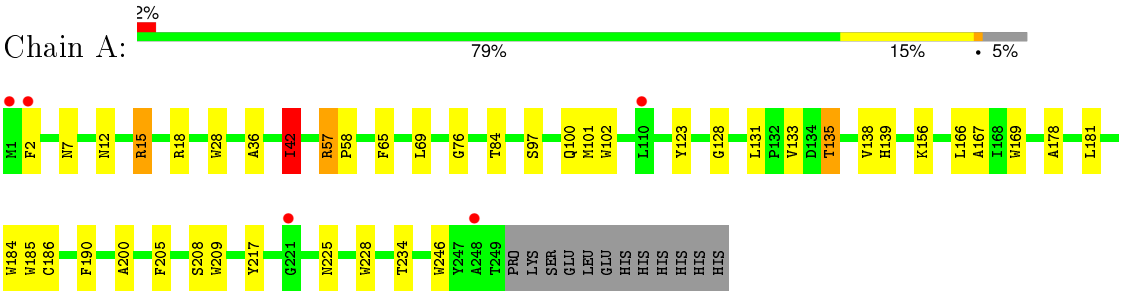
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	38	Total O 38 38	0	0
3	B	22	Total O 22 22	0	0
3	C	11	Total O 11 11	0	0
3	D	13	Total O 13 13	0	0
3	E	15	Total O 15 15	0	0
3	F	13	Total O 13 13	0	0
3	G	11	Total O 11 11	0	0
3	H	17	Total O 17 17	0	0
3	I	40	Total O 40 40	0	0
3	J	16	Total O 16 16	0	0

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

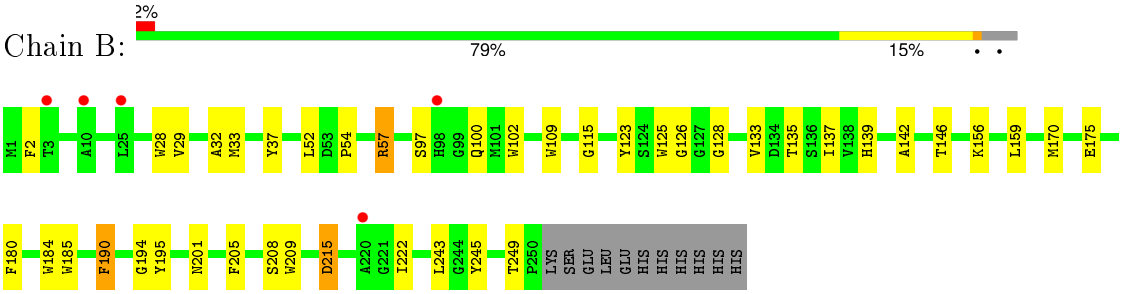
- Molecule 1: Nitrite transporter NirC

Chain A:



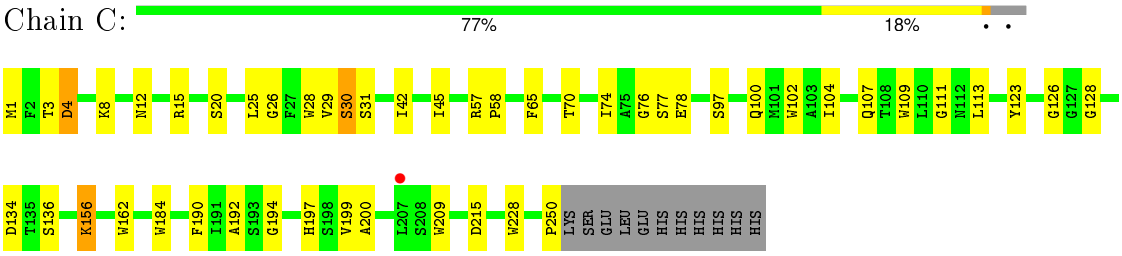
- Molecule 1: Nitrite transporter NirC

Chain B:



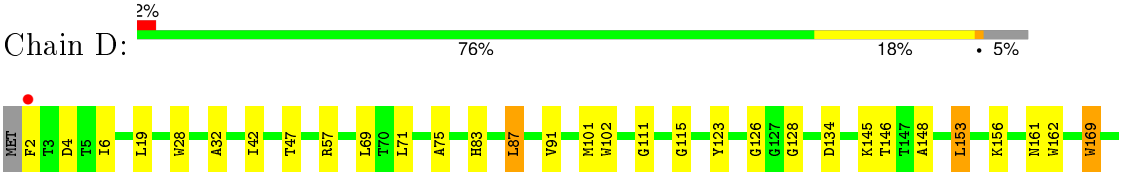
- Molecule 1: Nitrite transporter NirC

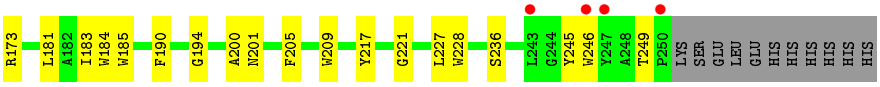
Chain C:



- Molecule 1: Nitrite transporter NirC

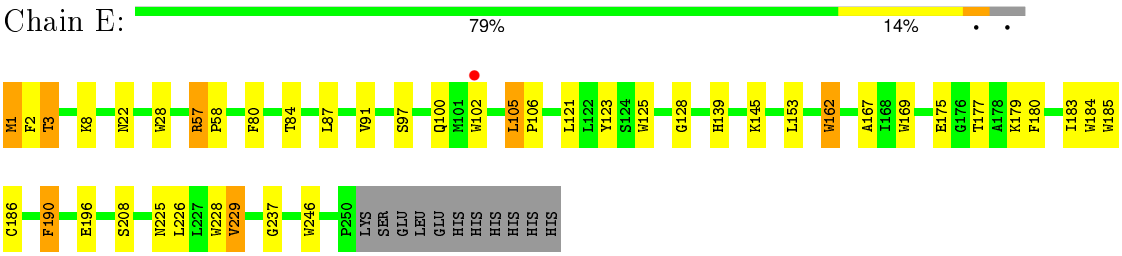
Chain D:





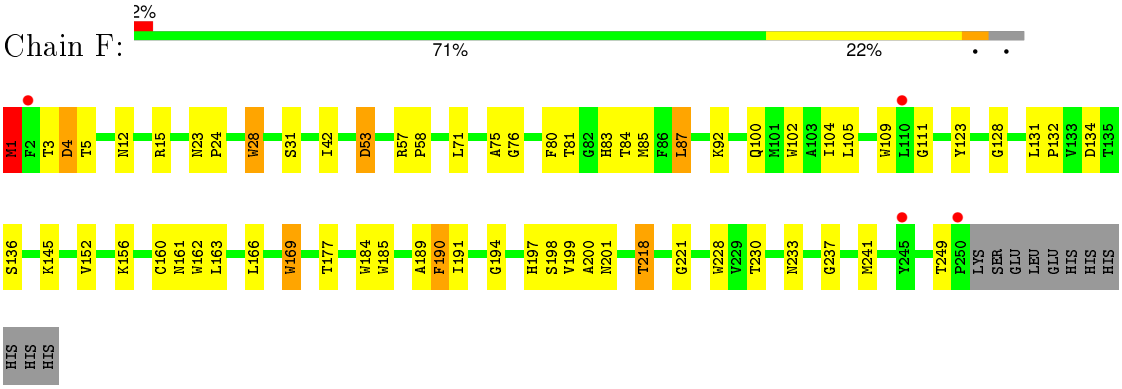
• Molecule 1: Nitrite transporter NirC

Chain E:



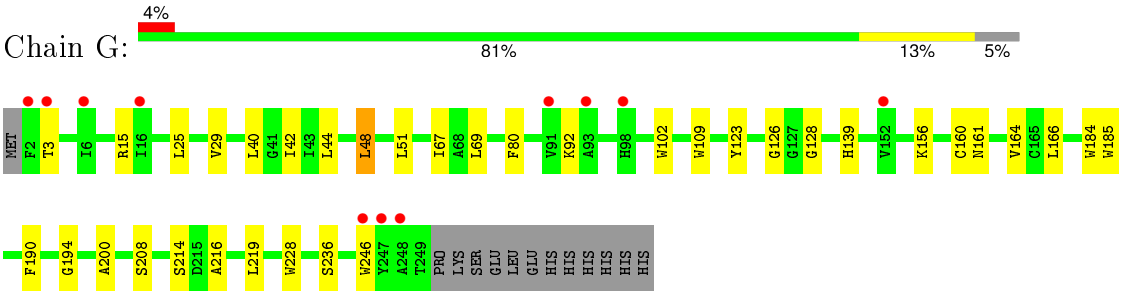
• Molecule 1: Nitrite transporter NirC

Chain F:



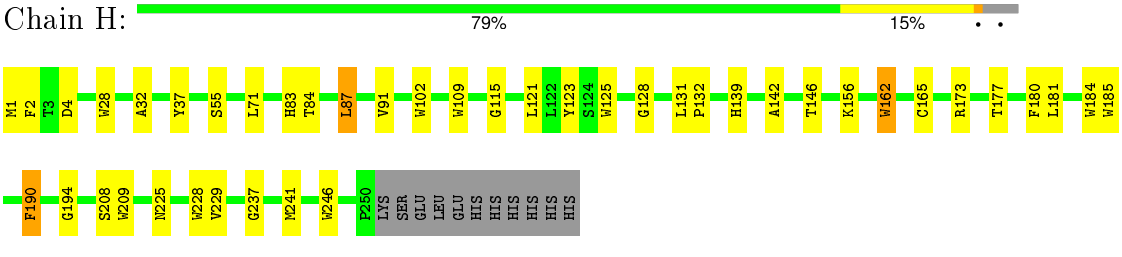
• Molecule 1: Nitrite transporter NirC

Chain G:



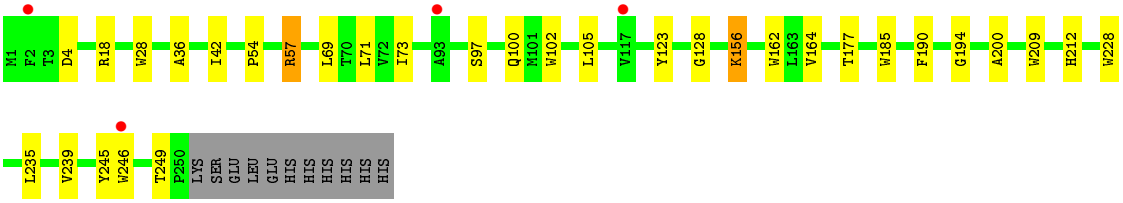
• Molecule 1: Nitrite transporter NirC

Chain H:

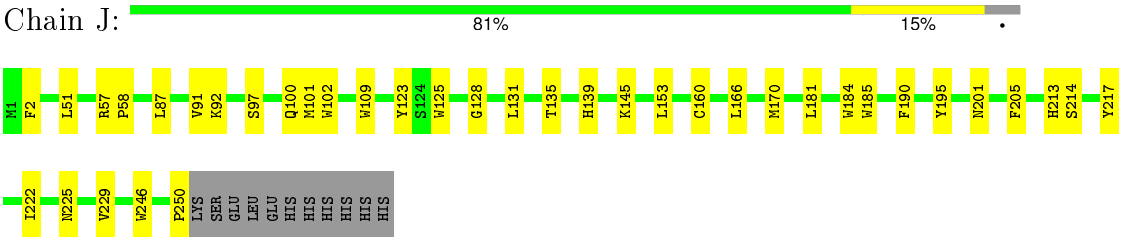


• Molecule 1: Nitrite transporter NirC

Chain I:



- Molecule 1: Nitrite transporter NirC



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	176.30Å 101.84Å 205.30Å 90.00° 101.24° 90.00°	Depositor
Resolution (Å)	87.75 – 2.40 87.75 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.2 (87.75-2.40) 97.1 (87.75-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.192 , 0.236 0.192 , 0.235	Depositor DCC
R_{free} test set	6772 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	45.6	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 39.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 135439 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19016	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.87% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: BOG

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	1.13	8/1928 (0.4%)	1.04	8/2638 (0.3%)
1	B	1.02	7/1936 (0.4%)	0.84	0/2650
1	C	0.98	7/1936 (0.4%)	0.87	3/2650 (0.1%)
1	D	0.95	9/1928 (0.5%)	0.84	1/2640 (0.0%)
1	E	1.08	10/1936 (0.5%)	0.94	1/2650 (0.0%)
1	F	1.03	7/1936 (0.4%)	0.91	3/2650 (0.1%)
1	G	0.98	6/1920 (0.3%)	0.87	2/2628 (0.1%)
1	H	1.11	10/1936 (0.5%)	0.94	0/2650
1	I	1.12	7/1936 (0.4%)	0.98	3/2650 (0.1%)
1	J	1.02	6/1936 (0.3%)	0.87	0/2650
All	All	1.04	77/19328 (0.4%)	0.91	21/26456 (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	F	0	1

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	185	TRP	CD2-CE2	7.84	1.50	1.41
1	A	185	TRP	CD2-CE2	7.47	1.50	1.41
1	H	209	TRP	CD2-CE2	7.32	1.50	1.41
1	H	162	TRP	CD2-CE2	6.92	1.49	1.41
1	F	169	TRP	CD2-CE2	6.83	1.49	1.41
1	E	228	TRP	CD2-CE2	6.76	1.49	1.41
1	E	28	TRP	CD2-CE2	6.69	1.49	1.41
1	B	125	TRP	CD2-CE2	6.64	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	28	TRP	CD2-CE2	6.62	1.49	1.41
1	C	109	TRP	CD2-CE2	6.60	1.49	1.41
1	G	184	TRP	CD2-CE2	6.58	1.49	1.41
1	H	28	TRP	CD2-CE2	6.53	1.49	1.41
1	H	228	TRP	CD2-CE2	6.52	1.49	1.41
1	I	228	TRP	CD2-CE2	6.49	1.49	1.41
1	B	209	TRP	CD2-CE2	6.46	1.49	1.41
1	F	102	TRP	CD2-CE2	6.39	1.49	1.41
1	B	185	TRP	CD2-CE2	6.31	1.49	1.41
1	G	246	TRP	CD2-CE2	6.28	1.48	1.41
1	F	162	TRP	CD2-CE2	6.25	1.48	1.41
1	D	162	TRP	CD2-CE2	6.23	1.48	1.41
1	E	102	TRP	CD2-CE2	6.23	1.48	1.41
1	J	184	TRP	CD2-CE2	6.22	1.48	1.41
1	A	246	TRP	CD2-CE2	6.22	1.48	1.41
1	C	28	TRP	CD2-CE2	6.21	1.48	1.41
1	C	184	TRP	CD2-CE2	6.19	1.48	1.41
1	E	185	TRP	CD2-CE2	6.18	1.48	1.41
1	D	246	TRP	CD2-CE2	6.16	1.48	1.41
1	E	169	TRP	CD2-CE2	6.12	1.48	1.41
1	E	246	TRP	CD2-CE2	6.12	1.48	1.41
1	D	28	TRP	CD2-CE2	6.10	1.48	1.41
1	H	246	TRP	CD2-CE2	6.06	1.48	1.41
1	A	209	TRP	CD2-CE2	6.05	1.48	1.41
1	E	162	TRP	CD2-CE2	6.02	1.48	1.41
1	D	209	TRP	CD2-CE2	6.02	1.48	1.41
1	I	246	TRP	CD2-CE2	5.97	1.48	1.41
1	H	125	TRP	CD2-CE2	5.85	1.48	1.41
1	D	228	TRP	CD2-CE2	5.83	1.48	1.41
1	F	109	TRP	CD2-CE2	5.83	1.48	1.41
1	H	185	TRP	CD2-CE2	5.82	1.48	1.41
1	A	28	TRP	CD2-CE2	5.79	1.48	1.41
1	J	102	TRP	CD2-CE2	5.79	1.48	1.41
1	G	228	TRP	CD2-CE2	5.78	1.48	1.41
1	H	109	TRP	CD2-CE2	5.78	1.48	1.41
1	D	169	TRP	CD2-CE2	5.74	1.48	1.41
1	B	28	TRP	CD2-CE2	5.73	1.48	1.41
1	E	184	TRP	CG-CD2	5.73	1.53	1.43
1	B	184	TRP	CD2-CE2	5.72	1.48	1.41
1	D	102	TRP	CD2-CE2	5.68	1.48	1.41
1	F	228	TRP	CD2-CE2	5.65	1.48	1.41
1	B	102	TRP	CD2-CE2	5.65	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	209	TRP	CD2-CE2	5.64	1.48	1.41
1	C	209	TRP	CD2-CE2	5.63	1.48	1.41
1	C	228	TRP	CD2-CE2	5.63	1.48	1.41
1	G	185	TRP	CD2-CE2	5.62	1.48	1.41
1	D	184	TRP	CD2-CE2	5.62	1.48	1.41
1	A	169	TRP	CD2-CE2	5.53	1.48	1.41
1	G	102	TRP	CD2-CE2	5.53	1.48	1.41
1	C	162	TRP	CD2-CE2	5.48	1.48	1.41
1	C	102	TRP	CD2-CE2	5.47	1.48	1.41
1	H	184	TRP	CG-CD2	5.46	1.52	1.43
1	G	109	TRP	CD2-CE2	5.39	1.47	1.41
1	J	246	TRP	CD2-CE2	5.38	1.47	1.41
1	F	28	TRP	CD2-CE2	5.38	1.47	1.41
1	A	228	TRP	CD2-CE2	5.37	1.47	1.41
1	B	109	TRP	CD2-CE2	5.35	1.47	1.41
1	E	125	TRP	CD2-CE2	5.34	1.47	1.41
1	A	184	TRP	CD2-CE2	5.33	1.47	1.41
1	I	185	TRP	CD2-CE2	5.21	1.47	1.41
1	I	102	TRP	CD2-CE2	5.13	1.47	1.41
1	E	184	TRP	CD2-CE2	5.11	1.47	1.41
1	J	125	TRP	CD2-CE2	5.10	1.47	1.41
1	A	102	TRP	CD2-CE2	5.10	1.47	1.41
1	F	184	TRP	CD2-CE2	5.10	1.47	1.41
1	D	185	TRP	CD2-CE2	5.03	1.47	1.41
1	J	109	TRP	CD2-CE2	5.03	1.47	1.41
1	H	102	TRP	CD2-CE2	5.02	1.47	1.41
1	I	162	TRP	CD2-CE2	5.00	1.47	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	15	ARG	NE-CZ-NH1	-11.17	114.71	120.30
1	A	15	ARG	NE-CZ-NH2	8.27	124.43	120.30
1	A	42	ILE	CG1-CB-CG2	-8.20	93.37	111.40
1	I	18	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	I	156	LYS	CD-CE-NZ	-7.92	93.49	111.70
1	D	57	ARG	NE-CZ-NH1	-7.78	116.41	120.30
1	A	18	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	C	134	ASP	CB-CG-OD1	6.95	124.55	118.30
1	A	18	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	E	57	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	G	48	LEU	CA-CB-CG	6.36	129.93	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	156	LYS	CD-CE-NZ	-6.15	97.55	111.70
1	I	4	ASP	CB-CG-OD2	6.07	123.77	118.30
1	F	53	ASP	CB-CA-C	-5.98	98.44	110.40
1	F	134	ASP	CB-CG-OD1	5.76	123.48	118.30
1	A	181	LEU	CA-CB-CG	5.53	128.01	115.30
1	A	101	MET	CG-SD-CE	5.50	109.00	100.20
1	G	15	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	F	53	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	C	215	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	57	ARG	NE-CZ-NH1	5.05	122.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	1	MET	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1874	0	1899	23	0
1	B	1881	0	1906	33	0
1	C	1881	0	1906	31	0
1	D	1873	0	1894	30	0
1	E	1881	0	1906	31	0
1	F	1881	0	1906	44	0
1	G	1866	0	1887	15	0
1	H	1881	0	1906	28	0
1	I	1881	0	1906	17	0
1	J	1881	0	1906	24	0
2	F	40	0	56	0	0
3	A	38	0	0	0	0
3	B	22	0	0	0	0
3	C	11	0	0	0	0
3	D	13	0	0	0	0
3	E	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	13	0	0	0	0
3	G	11	0	0	1	0
3	H	17	0	0	1	0
3	I	40	0	0	2	0
3	J	16	0	0	0	0
All	All	19016	0	19078	242	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 6.

All (242) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:MET:HE3	1:C:74:ILE:HB	1.21	1.15
1:B:170:MET:CE	1:C:74:ILE:HB	1.81	1.09
1:F:218:THR:HG22	1:F:221:GLY:H	1.01	1.08
1:C:12:ASN:OD1	1:C:15:ARG:NH2	1.95	0.99
1:E:97:SER:H	1:E:100:GLN:HE21	1.12	0.97
1:J:91:VAL:HG21	1:J:101:MET:HE3	1.44	0.97
1:J:97:SER:H	1:J:100:GLN:HE21	1.16	0.92
1:B:170:MET:HE3	1:C:74:ILE:CB	1.99	0.92
1:F:218:THR:HG22	1:F:221:GLY:N	1.86	0.91
1:H:1:MET:HA	1:H:173:ARG:NH1	1.86	0.91
1:B:97:SER:H	1:B:100:GLN:HE21	1.12	0.90
1:F:218:THR:CG2	1:F:221:GLY:H	1.87	0.86
1:J:91:VAL:HG21	1:J:101:MET:CE	2.05	0.85
1:J:91:VAL:CG2	1:J:101:MET:CE	2.57	0.82
1:F:198:SER:H	1:F:233:ASN:HD21	1.26	0.82
1:B:133:VAL:HG12	1:B:135:THR:HG22	1.60	0.81
1:E:80:PHE:HE1	1:E:105:LEU:HD23	1.44	0.80
1:E:80:PHE:CE1	1:E:105:LEU:HD23	2.18	0.78
1:A:131:LEU:O	1:A:139:HIS:HE1	1.66	0.78
1:E:97:SER:H	1:E:100:GLN:NE2	1.82	0.78
1:H:181:LEU:CD1	1:I:177:THR:HG23	2.14	0.77
1:F:160:CYS:SG	1:F:197:HIS:HB2	2.24	0.77
1:H:1:MET:HA	1:H:173:ARG:HH12	1.51	0.74
1:F:12:ASN:OD1	1:F:15:ARG:NH2	2.19	0.74
1:C:100:GLN:O	1:C:104:ILE:HG12	1.86	0.73
1:A:12:ASN:OD1	1:A:15:ARG:NH2	2.21	0.72
1:J:97:SER:H	1:J:100:GLN:NE2	1.86	0.71
1:H:181:LEU:HD11	1:I:177:THR:HG23	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:VAL:CG1	1:B:135:THR:HG22	2.21	0.70
1:C:25:LEU:O	1:C:29:VAL:HG12	1.90	0.70
1:F:81:THR:HB	1:F:161:ASN:ND2	2.08	0.69
1:B:97:SER:H	1:B:100:GLN:NE2	1.89	0.68
1:A:42:ILE:HD12	1:A:65:PHE:CE1	2.29	0.68
1:E:139:HIS:HD2	1:E:208:SER:OG	1.77	0.67
1:D:2:PHE:HD2	1:D:249:THR:HG22	1.60	0.67
1:C:42:ILE:HD11	1:C:200:ALA:HB1	1.77	0.66
1:F:57:ARG:HB3	1:F:58:PRO:HD3	1.77	0.66
1:B:170:MET:HE3	1:C:74:ILE:CG2	2.27	0.65
1:E:3:THR:HG21	1:H:4:ASP:OD1	1.97	0.64
1:F:123:TYR:CE2	1:F:128:GLY:HA3	2.33	0.64
1:C:31:SER:HB3	1:C:111:GLY:HA3	1.78	0.64
1:H:181:LEU:HD11	1:I:177:THR:CG2	2.28	0.63
1:H:142:ALA:O	1:H:146:THR:HG23	1.99	0.63
1:C:123:TYR:CE2	1:C:128:GLY:HA3	2.33	0.63
1:I:212:HIS:HD2	3:I:324:HOH:O	1.82	0.62
1:F:85:MET:HE1	1:F:169:TRP:CE3	2.35	0.62
1:H:139:HIS:HD2	1:H:208:SER:OG	1.82	0.62
1:I:54:PRO:HA	1:I:57:ARG:HG3	1.81	0.62
1:E:225:ASN:O	1:E:229:VAL:CG1	2.48	0.62
1:A:42:ILE:CD1	1:A:200:ALA:HB1	2.30	0.61
1:G:156:LYS:HE3	1:G:194:GLY:O	2.00	0.61
1:D:156:LYS:HD3	1:D:194:GLY:O	2.00	0.61
1:H:83:HIS:HB3	1:H:87:LEU:HD22	1.82	0.61
1:F:31:SER:HB3	1:F:111:GLY:HA3	1.81	0.61
1:B:156:LYS:HD2	1:C:126:GLY:O	2.01	0.61
1:E:225:ASN:O	1:E:229:VAL:HG12	2.02	0.60
1:B:170:MET:HE1	1:C:70:THR:HG22	1.83	0.60
1:J:91:VAL:HG23	1:J:101:MET:HE2	1.82	0.60
1:B:215:ASP:OD1	1:B:215:ASP:N	2.33	0.59
1:H:181:LEU:HD12	1:I:177:THR:HG23	1.84	0.59
1:J:87:LEU:HB3	1:J:101:MET:HG3	1.84	0.59
1:E:123:TYR:CE1	1:E:128:GLY:HA3	2.37	0.59
1:D:123:TYR:CZ	1:D:128:GLY:HA3	2.38	0.59
1:J:91:VAL:CG2	1:J:101:MET:HE2	2.33	0.59
1:D:148:ALA:HB3	1:D:153:LEU:CD1	2.33	0.58
1:C:15:ARG:NH1	1:C:78:GLU:OE2	2.37	0.58
1:D:71:LEU:O	1:D:75:ALA:HB3	2.03	0.58
1:C:30:SER:HB3	1:C:78:GLU:HG2	1.85	0.57
1:B:139:HIS:HD2	1:B:208:SER:OG	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:PRO:HG3	1:D:19:LEU:CD1	2.35	0.57
1:D:6:ILE:HD12	1:D:249:THR:HG21	1.85	0.57
1:I:69:LEU:HG	1:I:73:ILE:HD12	1.86	0.57
1:C:250:PRO:HG3	1:D:19:LEU:HD13	1.88	0.56
1:A:133:VAL:HG12	1:A:135:THR:HG22	1.88	0.56
1:A:42:ILE:HD12	1:A:65:PHE:HE1	1.70	0.55
1:F:156:LYS:HE2	1:G:126:GLY:O	2.05	0.55
1:F:1:MET:N	1:F:5:THR:H	2.04	0.55
1:F:185:TRP:HB3	1:G:67:ILE:HD12	1.87	0.55
1:D:181:LEU:HD12	1:E:177:THR:HG23	1.90	0.54
1:G:69:LEU:HD22	1:G:164:VAL:HG13	1.88	0.54
1:B:123:TYR:CZ	1:B:128:GLY:HA3	2.42	0.54
1:J:123:TYR:CZ	1:J:128:GLY:HA3	2.42	0.54
1:I:97:SER:H	1:I:100:GLN:HE21	1.54	0.54
1:B:156:LYS:HE3	1:B:194:GLY:O	2.09	0.53
1:J:145:LYS:NZ	1:J:201:ASN:HD21	2.07	0.53
1:F:177:THR:HG23	1:J:181:LEU:HD22	1.89	0.53
1:F:1:MET:HG2	1:F:4:ASP:H	1.74	0.53
1:C:20:SER:OG	1:C:107:GLN:NE2	2.41	0.53
1:C:123:TYR:CZ	1:C:128:GLY:HA3	2.44	0.52
1:G:42:ILE:HD11	1:G:200:ALA:HB1	1.91	0.52
1:G:139:HIS:HD2	1:G:208:SER:OG	1.92	0.52
1:D:145:LYS:NZ	1:D:201:ASN:HD21	2.06	0.52
1:A:2:PHE:HD2	1:A:7:ASN:HD21	1.58	0.52
1:D:148:ALA:HB3	1:D:153:LEU:HD11	1.90	0.52
1:G:123:TYR:CZ	1:G:128:GLY:HA3	2.45	0.51
1:D:169:TRP:O	1:D:173:ARG:HG3	2.10	0.51
1:E:87:LEU:O	1:E:91:VAL:HG23	2.11	0.51
1:A:166:LEU:HD21	1:B:37:TYR:CZ	2.46	0.51
1:A:156:LYS:HE3	1:B:126:GLY:O	2.11	0.51
1:B:142:ALA:O	1:B:146:THR:HG23	2.11	0.51
1:E:80:PHE:CE1	1:E:105:LEU:CD2	2.93	0.50
1:A:42:ILE:HD13	1:A:200:ALA:HB1	1.92	0.50
1:F:85:MET:HE3	1:F:241:MET:HB3	1.93	0.50
1:B:57:ARG:NH1	1:B:137:ILE:HG21	2.26	0.50
1:G:214:SER:HB3	1:G:216:ALA:H	1.77	0.50
1:G:214:SER:HB2	3:G:310:HOH:O	2.12	0.50
1:F:83:HIS:HB3	1:F:87:LEU:HD22	1.94	0.50
1:J:153:LEU:HD13	1:J:225:ASN:HA	1.93	0.49
1:E:167:ALA:HB2	1:E:186:CYS:HB2	1.94	0.49
1:F:123:TYR:CZ	1:F:128:GLY:HA3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:163:LEU:HG	1:G:40:LEU:HD13	1.93	0.49
1:B:170:MET:CE	1:C:74:ILE:CB	2.68	0.49
1:F:198:SER:OG	1:F:233:ASN:ND2	2.46	0.49
1:J:57:ARG:HB2	1:J:58:PRO:HD3	1.95	0.49
1:D:2:PHE:CD2	1:D:249:THR:HG22	2.44	0.48
1:J:201:ASN:HB3	1:J:205:PHE:CE2	2.47	0.48
1:D:161:ASN:HB3	1:D:236:SER:OG	2.12	0.48
1:I:156:LYS:HE3	1:I:194:GLY:O	2.13	0.48
1:E:190:PHE:C	1:E:190:PHE:CD1	2.86	0.48
1:B:2:PHE:HB2	1:B:249:THR:HG22	1.95	0.48
1:D:83:HIS:HB3	1:D:87:LEU:HD22	1.95	0.48
1:I:123:TYR:CE2	1:I:128:GLY:HA3	2.49	0.48
1:B:170:MET:CE	1:C:74:ILE:CG2	2.91	0.48
1:F:152:VAL:CG1	1:F:156:LYS:HE3	2.44	0.48
1:H:123:TYR:CE2	1:H:128:GLY:HA3	2.48	0.48
1:A:97:SER:H	1:A:100:GLN:HE21	1.62	0.47
1:I:42:ILE:HD11	1:I:200:ALA:HB1	1.95	0.47
1:C:57:ARG:HB2	1:C:58:PRO:HD3	1.95	0.47
1:A:139:HIS:HD2	1:A:208:SER:OG	1.96	0.47
1:F:197:HIS:CE1	1:F:199:VAL:HB	2.50	0.47
1:A:42:ILE:HD11	1:A:200:ALA:HB1	1.95	0.47
1:H:37:TYR:HB3	1:H:71:LEU:HB2	1.97	0.47
1:J:145:LYS:HZ1	1:J:201:ASN:HD21	1.63	0.47
1:F:145:LYS:NZ	1:F:201:ASN:HD21	2.12	0.47
1:E:225:ASN:OD1	1:E:229:VAL:HG11	2.15	0.47
1:A:205:PHE:HA	1:A:217:TYR:OH	2.15	0.47
1:E:225:ASN:O	1:E:229:VAL:HG13	2.16	0.46
1:E:123:TYR:CZ	1:E:128:GLY:HA3	2.50	0.46
1:F:189:ALA:HA	1:G:44:LEU:HD13	1.97	0.46
1:D:32:ALA:HA	1:D:111:GLY:O	2.16	0.46
1:A:2:PHE:HB2	1:A:7:ASN:ND2	2.30	0.46
1:E:84:THR:OG1	1:E:237:GLY:HA3	2.16	0.46
1:J:225:ASN:O	1:J:229:VAL:HG23	2.15	0.46
1:E:1:MET:N	3:E:313:HOH:O	2.42	0.46
1:A:76:GLY:HA3	1:E:2:PHE:HE1	1.81	0.46
1:H:156:LYS:HE3	1:H:194:GLY:O	2.16	0.46
1:D:148:ALA:HB3	1:D:153:LEU:HD13	1.97	0.46
1:D:32:ALA:O	1:D:115:GLY:HA3	2.16	0.46
1:E:57:ARG:HB2	1:E:58:PRO:HD3	1.97	0.46
1:B:29:VAL:O	1:B:33:MET:HG3	2.15	0.46
1:B:2:PHE:HE1	1:C:76:GLY:HA3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:131:LEU:HB2	1:F:132:PRO:HD3	1.97	0.45
1:G:25:LEU:O	1:G:29:VAL:HG23	2.17	0.45
1:B:54:PRO:HA	1:B:57:ARG:HD3	1.99	0.45
1:D:134:ASP:N	1:D:134:ASP:OD1	2.49	0.45
1:E:1:MET:HG2	1:E:2:PHE:CZ	2.51	0.45
1:D:245:TYR:O	1:D:249:THR:HG23	2.17	0.45
1:C:4:ASP:O	1:C:8:LYS:HG3	2.17	0.45
1:E:3:THR:CG2	1:H:4:ASP:OD1	2.65	0.45
1:E:177:THR:O	1:E:180:PHE:HB2	2.16	0.45
1:A:57:ARG:HB2	1:A:58:PRO:HD3	1.99	0.45
1:J:160:CYS:HB2	1:J:195:TYR:HB3	1.99	0.45
1:A:123:TYR:CE2	1:A:128:GLY:HA3	2.52	0.45
1:C:97:SER:OG	1:C:100:GLN:HG3	2.17	0.45
1:D:201:ASN:HB3	1:D:205:PHE:CE2	2.52	0.45
1:H:162:TRP:CH2	1:I:36:ALA:HB1	2.52	0.45
1:B:52:LEU:O	1:B:57:ARG:NH2	2.41	0.44
1:F:84:THR:OG1	1:F:237:GLY:HA3	2.17	0.44
1:G:123:TYR:CE2	1:G:128:GLY:HA3	2.51	0.44
1:I:164:VAL:HG12	3:I:330:HOH:O	2.16	0.44
1:E:179:LYS:O	1:E:183:ILE:HD12	2.16	0.44
1:F:81:THR:HB	1:F:161:ASN:HD21	1.78	0.44
1:I:245:TYR:O	1:I:249:THR:HG23	2.18	0.44
1:D:87:LEU:HB3	1:D:101:MET:HG3	1.99	0.44
1:D:87:LEU:O	1:D:91:VAL:HG23	2.18	0.44
1:H:190:PHE:C	1:H:190:PHE:CD1	2.91	0.44
1:F:92:LYS:HA	1:F:92:LYS:HD3	1.71	0.44
1:F:1:MET:HB3	1:F:4:ASP:HB2	1.99	0.44
1:J:213:HIS:HD2	1:J:214:SER:O	2.01	0.43
1:J:217:TYR:CZ	1:J:222:ILE:HD11	2.53	0.43
1:E:226:LEU:HD23	1:E:226:LEU:HA	1.89	0.43
1:F:76:GLY:HA3	1:J:2:PHE:HE1	1.83	0.43
1:C:57:ARG:CB	1:C:58:PRO:HD3	2.48	0.43
1:G:166:LEU:HD13	1:H:71:LEU:HD22	2.01	0.43
1:I:235:LEU:O	1:I:239:VAL:HB	2.18	0.43
1:H:121:LEU:HA	1:H:121:LEU:HD23	1.81	0.43
1:J:92:LYS:HE2	1:J:92:LYS:HA	2.01	0.43
1:F:152:VAL:HG12	1:F:156:LYS:HE3	2.00	0.43
1:I:105:LEU:HD23	1:I:105:LEU:HA	1.87	0.43
1:H:87:LEU:O	1:H:91:VAL:HG23	2.18	0.43
1:C:156:LYS:HD3	1:C:194:GLY:O	2.19	0.43
1:E:153:LEU:HD13	1:E:225:ASN:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:166:LEU:HD23	1:F:166:LEU:HA	1.93	0.43
1:F:105:LEU:HA	1:F:105:LEU:HD23	1.71	0.43
1:B:245:TYR:O	1:B:249:THR:HG23	2.18	0.42
1:I:123:TYR:CZ	1:I:128:GLY:HA3	2.54	0.42
1:F:190:PHE:CD1	1:F:190:PHE:C	2.92	0.42
1:D:42:ILE:HD11	1:D:200:ALA:HB1	2.01	0.42
1:A:178:ALA:HB1	1:B:180:PHE:CE1	2.54	0.42
1:H:55:SER:HB3	3:H:313:HOH:O	2.18	0.42
1:E:175:GLU:HA	1:E:175:GLU:OE2	2.20	0.42
1:H:225:ASN:O	1:H:229:VAL:HG23	2.19	0.42
1:F:100:GLN:O	1:F:104:ILE:HD12	2.20	0.42
1:F:191:ILE:HD12	1:F:191:ILE:HG23	1.88	0.42
1:G:161:ASN:HB3	1:G:236:SER:OG	2.20	0.42
1:C:45:ILE:HD13	1:C:65:PHE:CD1	2.55	0.42
1:H:177:THR:O	1:H:180:PHE:HB2	2.20	0.42
1:B:57:ARG:NH1	1:B:137:ILE:CG2	2.83	0.42
1:H:84:THR:OG1	1:H:237:GLY:HA3	2.19	0.42
1:F:23:ASN:ND2	1:J:250:PRO:HA	2.35	0.42
1:E:145:LYS:NZ	1:E:196:GLU:OE2	2.52	0.42
1:A:36:ALA:HB1	1:E:162:TRP:CH2	2.56	0.41
1:H:165:CYS:CB	1:H:241:MET:HG3	2.50	0.41
1:J:131:LEU:O	1:J:139:HIS:HE1	2.03	0.41
1:C:156:LYS:HE2	1:D:126:GLY:O	2.20	0.41
1:F:80:PHE:CE2	1:F:230:THR:HG23	2.54	0.41
1:B:205:PHE:CD2	1:B:222:ILE:HG23	2.55	0.41
1:F:24:PRO:O	1:F:28:TRP:HD1	2.04	0.41
1:F:123:TYR:HE2	1:F:131:LEU:HD13	1.86	0.41
1:F:156:LYS:HD3	1:F:194:GLY:O	2.21	0.41
1:A:84:THR:HG21	1:A:234:THR:HA	2.02	0.41
1:J:166:LEU:O	1:J:170:MET:HG3	2.19	0.41
1:C:197:HIS:CE1	1:C:199:VAL:HB	2.55	0.41
1:D:69:LEU:HB3	1:D:183:ILE:HG23	2.02	0.41
1:B:32:ALA:O	1:B:115:GLY:HA3	2.20	0.41
1:F:71:LEU:O	1:F:75:ALA:HB3	2.20	0.41
1:D:123:TYR:CE2	1:D:128:GLY:HA3	2.55	0.41
1:F:42:ILE:HD11	1:F:200:ALA:HB1	2.02	0.41
1:A:131:LEU:O	1:A:139:HIS:CE1	2.58	0.41
1:H:32:ALA:O	1:H:115:GLY:HA3	2.20	0.41
1:B:159:LEU:HD13	1:B:195:TYR:CE1	2.56	0.41
1:H:165:CYS:HB3	1:H:241:MET:HG3	2.03	0.41
1:C:192:ALA:O	1:D:47:THR:HG21	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:GLY:HA2	1:C:29:VAL:CG1	2.50	0.40
1:E:1:MET:HB3	1:E:2:PHE:CD2	2.56	0.40
1:B:190:PHE:CD1	1:B:190:PHE:C	2.94	0.40
1:A:167:ALA:HB2	1:A:186:CYS:CB	2.51	0.40
1:B:201:ASN:HB3	1:B:205:PHE:CE2	2.56	0.40
1:H:131:LEU:H	1:H:132:PRO:HD3	1.86	0.40
1:D:146:THR:HB	1:D:221:GLY:HA3	2.03	0.40
1:H:1:MET:CA	1:H:173:ARG:HH12	2.28	0.40
1:D:205:PHE:HA	1:D:217:TYR:OH	2.21	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	247/261 (95%)	244 (99%)	3 (1%)	0	100	100
1	B	248/261 (95%)	242 (98%)	6 (2%)	0	100	100
1	C	248/261 (95%)	241 (97%)	6 (2%)	1 (0%)	39	56
1	D	247/261 (95%)	243 (98%)	4 (2%)	0	100	100
1	E	248/261 (95%)	238 (96%)	10 (4%)	0	100	100
1	F	248/261 (95%)	240 (97%)	8 (3%)	0	100	100
1	G	246/261 (94%)	240 (98%)	6 (2%)	0	100	100
1	H	248/261 (95%)	241 (97%)	6 (2%)	1 (0%)	39	56
1	I	248/261 (95%)	243 (98%)	5 (2%)	0	100	100
1	J	248/261 (95%)	243 (98%)	5 (2%)	0	100	100
All	All	2476/2610 (95%)	2415 (98%)	59 (2%)	2 (0%)	56	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	2	PHE
1	C	77	SER

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	191/203 (94%)	185 (97%)	6 (3%)	47 69
1	B	192/203 (95%)	187 (97%)	5 (3%)	54 74
1	C	192/203 (95%)	185 (96%)	7 (4%)	42 63
1	D	191/203 (94%)	186 (97%)	5 (3%)	54 74
1	E	192/203 (95%)	183 (95%)	9 (5%)	32 50
1	F	192/203 (95%)	183 (95%)	9 (5%)	32 50
1	G	190/203 (94%)	182 (96%)	8 (4%)	36 56
1	H	192/203 (95%)	190 (99%)	2 (1%)	82 93
1	I	192/203 (95%)	189 (98%)	3 (2%)	70 86
1	J	192/203 (95%)	189 (98%)	3 (2%)	70 86
All	All	1916/2030 (94%)	1859 (97%)	57 (3%)	48 70

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ILE
1	A	69	LEU
1	A	135	THR
1	A	138	VAL
1	A	190	PHE
1	A	225	ASN
1	B	57	ARG
1	B	175	GLU
1	B	190	PHE
1	B	215	ASP
1	B	243	LEU
1	C	1	MET

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Mol	Chain	Res	Type
1	C	3	THR
1	C	4	ASP
1	C	30	SER
1	C	113	LEU
1	C	136	SER
1	C	190	PHE
1	D	4	ASP
1	D	87	LEU
1	D	153	LEU
1	D	190	PHE
1	D	227	LEU
1	E	1	MET
1	E	3	THR
1	E	8	LYS
1	E	22	ASN
1	E	105	LEU
1	E	106	PRO
1	E	121	LEU
1	E	190	PHE
1	E	229	VAL
1	F	1	MET
1	F	3	THR
1	F	4	ASP
1	F	53	ASP
1	F	87	LEU
1	F	136	SER
1	F	190	PHE
1	F	218	THR
1	F	249	THR
1	G	3	THR
1	G	48	LEU
1	G	51	LEU
1	G	80	PHE
1	G	92	LYS
1	G	160	CYS
1	G	190	PHE
1	G	219	LEU
1	H	87	LEU
1	H	190	PHE
1	I	57	ARG
1	I	71	LEU
1	I	190	PHE

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Mol	Chain	Res	Type
1	J	51	LEU
1	J	135	THR
1	J	190	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	100	GLN
1	A	139	HIS
1	A	201	ASN
1	A	225	ASN
1	B	7	ASN
1	B	100	GLN
1	B	107	GLN
1	B	139	HIS
1	B	201	ASN
1	C	7	ASN
1	C	201	ASN
1	C	213	HIS
1	D	7	ASN
1	D	139	HIS
1	D	201	ASN
1	E	7	ASN
1	E	100	GLN
1	E	139	HIS
1	E	201	ASN
1	F	7	ASN
1	F	161	ASN
1	F	201	ASN
1	F	233	ASN
1	G	7	ASN
1	G	23	ASN
1	G	139	HIS
1	G	201	ASN
1	H	98	HIS
1	H	107	GLN
1	H	139	HIS
1	H	201	ASN
1	I	7	ASN
1	I	100	GLN
1	I	107	GLN

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Mol	Chain	Res	Type
1	I	201	ASN
1	I	212	HIS
1	J	7	ASN
1	J	100	GLN
1	J	139	HIS
1	J	201	ASN
1	J	213	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	BOG	F	301	-	20,20,20	1.15	2 (10%)	25,25,25	1.60	3 (12%)
2	BOG	F	302	-	20,20,20	1.34	2 (10%)	25,25,25	2.60	9 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BOG	F	301	-	-	0/11/31/31	0/1/1/1
2	BOG	F	302	-	-	0/11/31/31	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	BOG	O5-C1	2.11	1.47	1.41
2	F	302	BOG	O5-C1	2.26	1.47	1.41
2	F	301	BOG	O1-C1	3.20	1.45	1.40
2	F	302	BOG	O1-C1	3.74	1.46	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	301	BOG	C4-C3-C2	-2.69	105.78	110.79
2	F	302	BOG	C1-O5-C5	-2.57	108.76	113.75
2	F	302	BOG	O5-C1-O1	2.18	115.31	110.05
2	F	302	BOG	O6-C6-C5	2.26	118.80	111.33
2	F	301	BOG	O3-C3-C4	2.27	115.45	110.34
2	F	302	BOG	C6-C5-C4	2.97	120.35	113.02
2	F	302	BOG	O3-C3-C4	3.05	117.21	110.34
2	F	302	BOG	O5-C1-C2	3.11	116.66	110.28
2	F	302	BOG	O5-C5-C6	4.01	116.49	106.36
2	F	301	BOG	C1-O5-C5	4.70	122.86	113.75
2	F	302	BOG	C1'-O1-C1	6.60	125.49	113.94
2	F	302	BOG	O1-C1-C2	7.25	117.20	108.04

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, 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	249/261 (95%)	0.44	5 (2%) 68 68	31, 41, 55, 74	1 (0%)
1	B	250/261 (95%)	0.41	5 (2%) 68 68	33, 47, 66, 94	0
1	C	250/261 (95%)	0.43	1 (0%) 93 93	35, 52, 78, 107	0
1	D	249/261 (95%)	0.38	5 (2%) 68 68	36, 56, 77, 93	0
1	E	250/261 (95%)	0.34	1 (0%) 93 93	32, 48, 63, 73	0
1	F	250/261 (95%)	0.41	4 (1%) 74 74	32, 48, 71, 93	1 (0%)
1	G	248/261 (95%)	0.49	11 (4%) 38 39	34, 51, 69, 87	0
1	H	250/261 (95%)	0.39	0 100 100	34, 46, 60, 76	0
1	I	250/261 (95%)	0.47	4 (1%) 74 74	30, 40, 52, 101	0
1	J	250/261 (95%)	0.31	0 100 100	31, 46, 64, 90	0
All	All	2496/2610 (95%)	0.41	36 (1%) 78 77	30, 47, 69, 107	2 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	2	PHE	4.6
1	G	3	THR	4.5
1	G	246	TRP	4.0
1	F	2	PHE	4.0
1	A	248	ALA	3.4
1	G	2	PHE	3.3
1	D	250	PRO	3.3
1	B	3	THR	3.2
1	A	2	PHE	3.2
1	B	220	ALA	3.0
1	D	2	PHE	2.9
1	A	110	LEU	2.7
1	G	91	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	247	TYR	2.6
1	E	102	TRP	2.6
1	F	250	PRO	2.5
1	F	245	TYR	2.5
1	D	246	TRP	2.4
1	F	110	LEU	2.4
1	G	16	ILE	2.4
1	B	98	HIS	2.4
1	G	93	ALA	2.4
1	G	152	VAL	2.3
1	I	246	TRP	2.3
1	D	243	LEU	2.3
1	B	25	LEU	2.2
1	A	1	MET	2.2
1	G	248	ALA	2.2
1	B	10	ALA	2.2
1	C	207	LEU	2.2
1	A	221	GLY	2.2
1	D	247	TYR	2.1
1	G	6	ILE	2.1
1	G	98	HIS	2.1
1	I	93	ALA	2.0
1	I	117	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	BOG	F	302	20/20	0.65	0.29	4.53	54,83,114,116	0
2	BOG	F	301	20/20	0.61	0.24	-	53,90,108,114	0

6.5 Other polymers (i)

There are no such residues in this entry.