Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:33 PM GMT

PDB ID	:	3ZSF
Title	:	Crystal structure of the L-cystine solute receptor of Neisseria gonorrhoeae in the unliganded open conformation
Authors	:	Bulut, H.; Moniot, S.; Scheffel, F.; Gathmann, S.; Licht, A.; Saenger, W.; Schneider, E.
Deposited on	:	2011-06-27
Resolution	:	2.32 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:

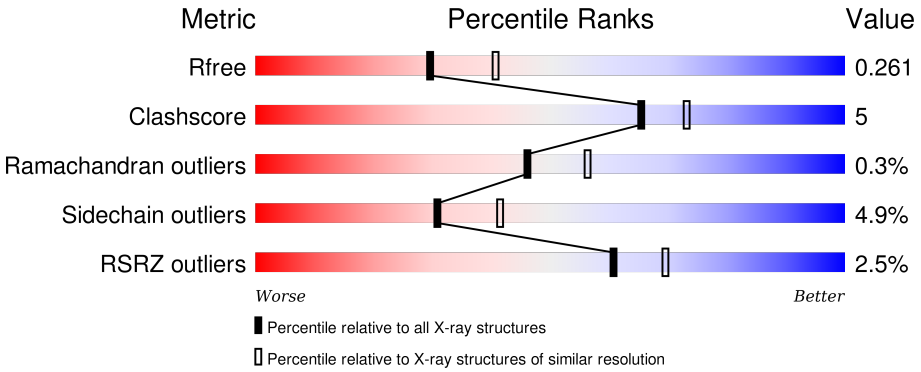
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.32 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	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

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	283	77% 6% 16%
1	B	283	6% 72% 9% • 16%
1	C	283	72% 11% 17%
1	D	283	% 73% 9% •• 16%
1	E	283	72% 12% 16%

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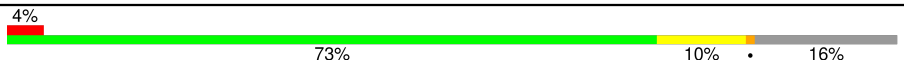
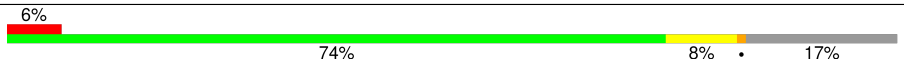
Mol	Chain	Length	Quality of chain
1	F	283	
1	G	283	
1	H	283	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14685 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 ABC TRANSPORTER, PERIPLASMIC BINDING PROTEIN, AMINO ACID.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	2	0
			1793	1128	302	361	2			
1	B	237	Total	C	N	O	S	0	1	0
			1756	1102	295	357	2			
1	C	235	Total	C	N	O	S	0	0	0
			1756	1106	297	351	2			
1	D	237	Total	C	N	O	S	0	0	0
			1763	1108	300	353	2			
1	E	237	Total	C	N	O	S	0	1	0
			1786	1124	302	357	3			
1	F	238	Total	C	N	O	S	0	1	0
			1757	1103	299	353	2			
1	G	235	Total	C	N	O	S	0	3	0
			1771	1115	299	355	2			
1	H	236	Total	C	N	O	S	0	0	0
			1724	1084	291	347	2			

There are 200 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	EXPRESSION TAG	UNP Q5F9M1
A	-6	GLY	-	EXPRESSION TAG	UNP Q5F9M1
A	-5	HIS	-	EXPRESSION TAG	UNP Q5F9M1
A	-4	HIS	-	EXPRESSION TAG	UNP Q5F9M1
A	-3	HIS	-	EXPRESSION TAG	UNP Q5F9M1
A	-2	HIS	-	EXPRESSION TAG	UNP Q5F9M1
A	-1	HIS	-	EXPRESSION TAG	UNP Q5F9M1
A	0	HIS	-	EXPRESSION TAG	UNP Q5F9M1
A	1	HIS	-	EXPRESSION TAG	UNP Q5F9M1
A	2	HIS	-	EXPRESSION TAG	UNP Q5F9M1
A	3	HIS	-	EXPRESSION TAG	UNP Q5F9M1
A	4	HIS	-	EXPRESSION TAG	UNP Q5F9M1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	5	SER	-	EXPRESSION TAG	UNP Q5F9M1
A	6	SER	-	EXPRESSION TAG	UNP Q5F9M1
A	7	GLY	-	EXPRESSION TAG	UNP Q5F9M1
A	8	HIS	-	EXPRESSION TAG	UNP Q5F9M1
A	9	ILE	-	EXPRESSION TAG	UNP Q5F9M1
A	10	ASP	-	EXPRESSION TAG	UNP Q5F9M1
A	11	ASP	-	EXPRESSION TAG	UNP Q5F9M1
A	12	ASP	-	EXPRESSION TAG	UNP Q5F9M1
A	13	ASP	-	EXPRESSION TAG	UNP Q5F9M1
A	14	LYS	-	EXPRESSION TAG	UNP Q5F9M1
A	15	HIS	-	EXPRESSION TAG	UNP Q5F9M1
A	16	MET	-	EXPRESSION TAG	UNP Q5F9M1
A	19	ALA	CYS	ENGINEERED MUTATION	UNP Q5F9M1
B	-7	MET	-	EXPRESSION TAG	UNP Q5F9M1
B	-6	GLY	-	EXPRESSION TAG	UNP Q5F9M1
B	-5	HIS	-	EXPRESSION TAG	UNP Q5F9M1
B	-4	HIS	-	EXPRESSION TAG	UNP Q5F9M1
B	-3	HIS	-	EXPRESSION TAG	UNP Q5F9M1
B	-2	HIS	-	EXPRESSION TAG	UNP Q5F9M1
B	-1	HIS	-	EXPRESSION TAG	UNP Q5F9M1
B	0	HIS	-	EXPRESSION TAG	UNP Q5F9M1
B	1	HIS	-	EXPRESSION TAG	UNP Q5F9M1
B	2	HIS	-	EXPRESSION TAG	UNP Q5F9M1
B	3	HIS	-	EXPRESSION TAG	UNP Q5F9M1
B	4	HIS	-	EXPRESSION TAG	UNP Q5F9M1
B	5	SER	-	EXPRESSION TAG	UNP Q5F9M1
B	6	SER	-	EXPRESSION TAG	UNP Q5F9M1
B	7	GLY	-	EXPRESSION TAG	UNP Q5F9M1
B	8	HIS	-	EXPRESSION TAG	UNP Q5F9M1
B	9	ILE	-	EXPRESSION TAG	UNP Q5F9M1
B	10	ASP	-	EXPRESSION TAG	UNP Q5F9M1
B	11	ASP	-	EXPRESSION TAG	UNP Q5F9M1
B	12	ASP	-	EXPRESSION TAG	UNP Q5F9M1
B	13	ASP	-	EXPRESSION TAG	UNP Q5F9M1
B	14	LYS	-	EXPRESSION TAG	UNP Q5F9M1
B	15	HIS	-	EXPRESSION TAG	UNP Q5F9M1
B	16	MET	-	EXPRESSION TAG	UNP Q5F9M1
B	19	ALA	CYS	ENGINEERED MUTATION	UNP Q5F9M1
C	-7	MET	-	EXPRESSION TAG	UNP Q5F9M1
C	-6	GLY	-	EXPRESSION TAG	UNP Q5F9M1
C	-5	HIS	-	EXPRESSION TAG	UNP Q5F9M1
C	-4	HIS	-	EXPRESSION TAG	UNP Q5F9M1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	HIS	-	EXPRESSION TAG	UNP Q5F9M1
C	-2	HIS	-	EXPRESSION TAG	UNP Q5F9M1
C	-1	HIS	-	EXPRESSION TAG	UNP Q5F9M1
C	0	HIS	-	EXPRESSION TAG	UNP Q5F9M1
C	1	HIS	-	EXPRESSION TAG	UNP Q5F9M1
C	2	HIS	-	EXPRESSION TAG	UNP Q5F9M1
C	3	HIS	-	EXPRESSION TAG	UNP Q5F9M1
C	4	HIS	-	EXPRESSION TAG	UNP Q5F9M1
C	5	SER	-	EXPRESSION TAG	UNP Q5F9M1
C	6	SER	-	EXPRESSION TAG	UNP Q5F9M1
C	7	GLY	-	EXPRESSION TAG	UNP Q5F9M1
C	8	HIS	-	EXPRESSION TAG	UNP Q5F9M1
C	9	ILE	-	EXPRESSION TAG	UNP Q5F9M1
C	10	ASP	-	EXPRESSION TAG	UNP Q5F9M1
C	11	ASP	-	EXPRESSION TAG	UNP Q5F9M1
C	12	ASP	-	EXPRESSION TAG	UNP Q5F9M1
C	13	ASP	-	EXPRESSION TAG	UNP Q5F9M1
C	14	LYS	-	EXPRESSION TAG	UNP Q5F9M1
C	15	HIS	-	EXPRESSION TAG	UNP Q5F9M1
C	16	MET	-	EXPRESSION TAG	UNP Q5F9M1
C	19	ALA	CYS	ENGINEERED MUTATION	UNP Q5F9M1
D	-7	MET	-	EXPRESSION TAG	UNP Q5F9M1
D	-6	GLY	-	EXPRESSION TAG	UNP Q5F9M1
D	-5	HIS	-	EXPRESSION TAG	UNP Q5F9M1
D	-4	HIS	-	EXPRESSION TAG	UNP Q5F9M1
D	-3	HIS	-	EXPRESSION TAG	UNP Q5F9M1
D	-2	HIS	-	EXPRESSION TAG	UNP Q5F9M1
D	-1	HIS	-	EXPRESSION TAG	UNP Q5F9M1
D	0	HIS	-	EXPRESSION TAG	UNP Q5F9M1
D	1	HIS	-	EXPRESSION TAG	UNP Q5F9M1
D	2	HIS	-	EXPRESSION TAG	UNP Q5F9M1
D	3	HIS	-	EXPRESSION TAG	UNP Q5F9M1
D	4	HIS	-	EXPRESSION TAG	UNP Q5F9M1
D	5	SER	-	EXPRESSION TAG	UNP Q5F9M1
D	6	SER	-	EXPRESSION TAG	UNP Q5F9M1
D	7	GLY	-	EXPRESSION TAG	UNP Q5F9M1
D	8	HIS	-	EXPRESSION TAG	UNP Q5F9M1
D	9	ILE	-	EXPRESSION TAG	UNP Q5F9M1
D	10	ASP	-	EXPRESSION TAG	UNP Q5F9M1
D	11	ASP	-	EXPRESSION TAG	UNP Q5F9M1
D	12	ASP	-	EXPRESSION TAG	UNP Q5F9M1
D	13	ASP	-	EXPRESSION TAG	UNP Q5F9M1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	14	LYS	-	EXPRESSION TAG	UNP Q5F9M1
D	15	HIS	-	EXPRESSION TAG	UNP Q5F9M1
D	16	MET	-	EXPRESSION TAG	UNP Q5F9M1
D	19	ALA	CYS	ENGINEERED MUTATION	UNP Q5F9M1
E	-7	MET	-	EXPRESSION TAG	UNP Q5F9M1
E	-6	GLY	-	EXPRESSION TAG	UNP Q5F9M1
E	-5	HIS	-	EXPRESSION TAG	UNP Q5F9M1
E	-4	HIS	-	EXPRESSION TAG	UNP Q5F9M1
E	-3	HIS	-	EXPRESSION TAG	UNP Q5F9M1
E	-2	HIS	-	EXPRESSION TAG	UNP Q5F9M1
E	-1	HIS	-	EXPRESSION TAG	UNP Q5F9M1
E	0	HIS	-	EXPRESSION TAG	UNP Q5F9M1
E	1	HIS	-	EXPRESSION TAG	UNP Q5F9M1
E	2	HIS	-	EXPRESSION TAG	UNP Q5F9M1
E	3	HIS	-	EXPRESSION TAG	UNP Q5F9M1
E	4	HIS	-	EXPRESSION TAG	UNP Q5F9M1
E	5	SER	-	EXPRESSION TAG	UNP Q5F9M1
E	6	SER	-	EXPRESSION TAG	UNP Q5F9M1
E	7	GLY	-	EXPRESSION TAG	UNP Q5F9M1
E	8	HIS	-	EXPRESSION TAG	UNP Q5F9M1
E	9	ILE	-	EXPRESSION TAG	UNP Q5F9M1
E	10	ASP	-	EXPRESSION TAG	UNP Q5F9M1
E	11	ASP	-	EXPRESSION TAG	UNP Q5F9M1
E	12	ASP	-	EXPRESSION TAG	UNP Q5F9M1
E	13	ASP	-	EXPRESSION TAG	UNP Q5F9M1
E	14	LYS	-	EXPRESSION TAG	UNP Q5F9M1
E	15	HIS	-	EXPRESSION TAG	UNP Q5F9M1
E	16	MET	-	EXPRESSION TAG	UNP Q5F9M1
E	19	ALA	CYS	ENGINEERED MUTATION	UNP Q5F9M1
F	-7	MET	-	EXPRESSION TAG	UNP Q5F9M1
F	-6	GLY	-	EXPRESSION TAG	UNP Q5F9M1
F	-5	HIS	-	EXPRESSION TAG	UNP Q5F9M1
F	-4	HIS	-	EXPRESSION TAG	UNP Q5F9M1
F	-3	HIS	-	EXPRESSION TAG	UNP Q5F9M1
F	-2	HIS	-	EXPRESSION TAG	UNP Q5F9M1
F	-1	HIS	-	EXPRESSION TAG	UNP Q5F9M1
F	0	HIS	-	EXPRESSION TAG	UNP Q5F9M1
F	1	HIS	-	EXPRESSION TAG	UNP Q5F9M1
F	2	HIS	-	EXPRESSION TAG	UNP Q5F9M1
F	3	HIS	-	EXPRESSION TAG	UNP Q5F9M1
F	4	HIS	-	EXPRESSION TAG	UNP Q5F9M1
F	5	SER	-	EXPRESSION TAG	UNP Q5F9M1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	6	SER	-	EXPRESSION TAG	UNP Q5F9M1
F	7	GLY	-	EXPRESSION TAG	UNP Q5F9M1
F	8	HIS	-	EXPRESSION TAG	UNP Q5F9M1
F	9	ILE	-	EXPRESSION TAG	UNP Q5F9M1
F	10	ASP	-	EXPRESSION TAG	UNP Q5F9M1
F	11	ASP	-	EXPRESSION TAG	UNP Q5F9M1
F	12	ASP	-	EXPRESSION TAG	UNP Q5F9M1
F	13	ASP	-	EXPRESSION TAG	UNP Q5F9M1
F	14	LYS	-	EXPRESSION TAG	UNP Q5F9M1
F	15	HIS	-	EXPRESSION TAG	UNP Q5F9M1
F	16	MET	-	EXPRESSION TAG	UNP Q5F9M1
F	19	ALA	CYS	ENGINEERED MUTATION	UNP Q5F9M1
G	-7	MET	-	EXPRESSION TAG	UNP Q5F9M1
G	-6	GLY	-	EXPRESSION TAG	UNP Q5F9M1
G	-5	HIS	-	EXPRESSION TAG	UNP Q5F9M1
G	-4	HIS	-	EXPRESSION TAG	UNP Q5F9M1
G	-3	HIS	-	EXPRESSION TAG	UNP Q5F9M1
G	-2	HIS	-	EXPRESSION TAG	UNP Q5F9M1
G	-1	HIS	-	EXPRESSION TAG	UNP Q5F9M1
G	0	HIS	-	EXPRESSION TAG	UNP Q5F9M1
G	1	HIS	-	EXPRESSION TAG	UNP Q5F9M1
G	2	HIS	-	EXPRESSION TAG	UNP Q5F9M1
G	3	HIS	-	EXPRESSION TAG	UNP Q5F9M1
G	4	HIS	-	EXPRESSION TAG	UNP Q5F9M1
G	5	SER	-	EXPRESSION TAG	UNP Q5F9M1
G	6	SER	-	EXPRESSION TAG	UNP Q5F9M1
G	7	GLY	-	EXPRESSION TAG	UNP Q5F9M1
G	8	HIS	-	EXPRESSION TAG	UNP Q5F9M1
G	9	ILE	-	EXPRESSION TAG	UNP Q5F9M1
G	10	ASP	-	EXPRESSION TAG	UNP Q5F9M1
G	11	ASP	-	EXPRESSION TAG	UNP Q5F9M1
G	12	ASP	-	EXPRESSION TAG	UNP Q5F9M1
G	13	ASP	-	EXPRESSION TAG	UNP Q5F9M1
G	14	LYS	-	EXPRESSION TAG	UNP Q5F9M1
G	15	HIS	-	EXPRESSION TAG	UNP Q5F9M1
G	16	MET	-	EXPRESSION TAG	UNP Q5F9M1
G	19	ALA	CYS	ENGINEERED MUTATION	UNP Q5F9M1
H	-7	MET	-	EXPRESSION TAG	UNP Q5F9M1
H	-6	GLY	-	EXPRESSION TAG	UNP Q5F9M1
H	-5	HIS	-	EXPRESSION TAG	UNP Q5F9M1
H	-4	HIS	-	EXPRESSION TAG	UNP Q5F9M1
H	-3	HIS	-	EXPRESSION TAG	UNP Q5F9M1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	HIS	-	EXPRESSION TAG	UNP Q5F9M1
H	-1	HIS	-	EXPRESSION TAG	UNP Q5F9M1
H	0	HIS	-	EXPRESSION TAG	UNP Q5F9M1
H	1	HIS	-	EXPRESSION TAG	UNP Q5F9M1
H	2	HIS	-	EXPRESSION TAG	UNP Q5F9M1
H	3	HIS	-	EXPRESSION TAG	UNP Q5F9M1
H	4	HIS	-	EXPRESSION TAG	UNP Q5F9M1
H	5	SER	-	EXPRESSION TAG	UNP Q5F9M1
H	6	SER	-	EXPRESSION TAG	UNP Q5F9M1
H	7	GLY	-	EXPRESSION TAG	UNP Q5F9M1
H	8	HIS	-	EXPRESSION TAG	UNP Q5F9M1
H	9	ILE	-	EXPRESSION TAG	UNP Q5F9M1
H	10	ASP	-	EXPRESSION TAG	UNP Q5F9M1
H	11	ASP	-	EXPRESSION TAG	UNP Q5F9M1
H	12	ASP	-	EXPRESSION TAG	UNP Q5F9M1
H	13	ASP	-	EXPRESSION TAG	UNP Q5F9M1
H	14	LYS	-	EXPRESSION TAG	UNP Q5F9M1
H	15	HIS	-	EXPRESSION TAG	UNP Q5F9M1
H	16	MET	-	EXPRESSION TAG	UNP Q5F9M1
H	19	ALA	CYS	ENGINEERED MUTATION	UNP Q5F9M1

- Molecule 2 is water.

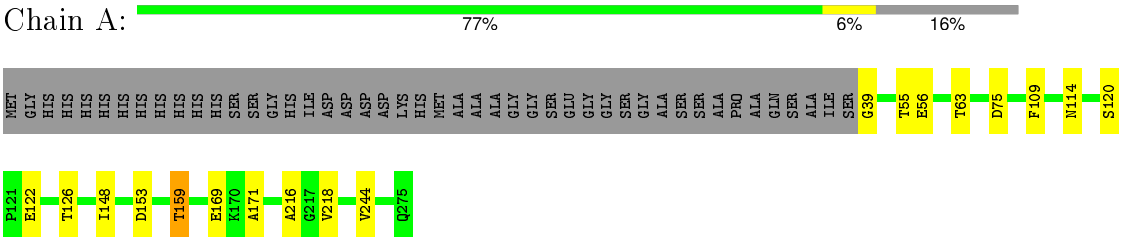
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	83	Total O 83 83	0	0
2	B	60	Total O 60 60	0	0
2	C	74	Total O 74 74	0	0
2	D	63	Total O 63 63	0	0
2	E	85	Total O 85 85	0	0
2	F	64	Total O 64 64	0	0
2	G	83	Total O 83 83	0	0
2	H	67	Total O 67 67	0	0

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.

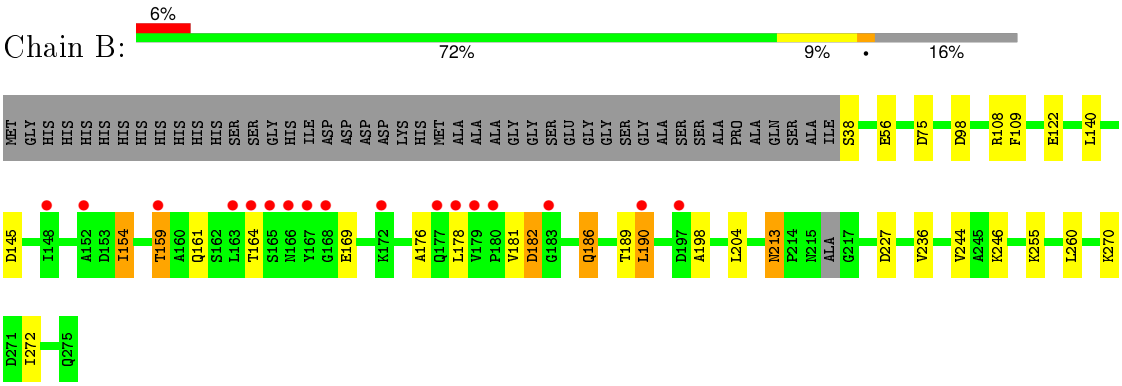
• Molecule 1: ABC TRANSPORTER, PERIPLASMIC BINDING PROTEIN, AMINO ACID

Chain A:



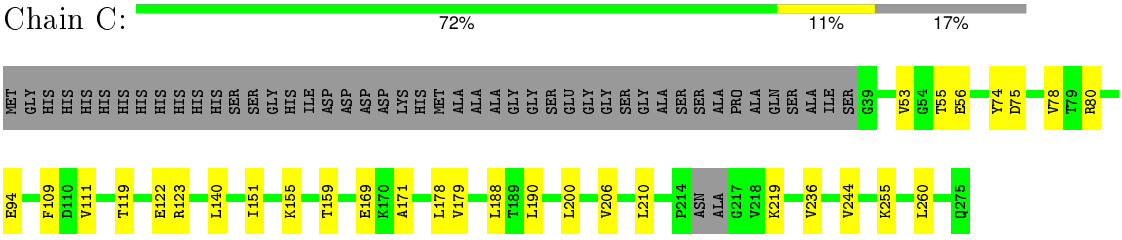
• Molecule 1: ABC TRANSPORTER, PERIPLASMIC BINDING PROTEIN, AMINO ACID

Chain B:



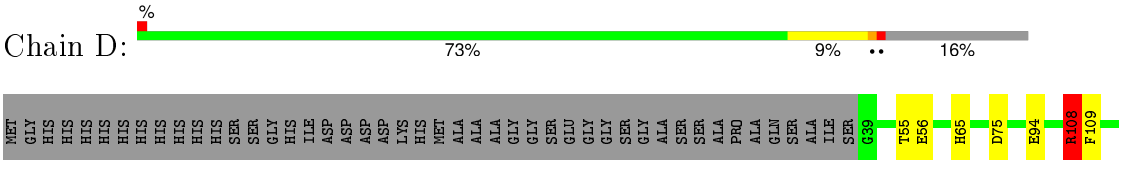
• Molecule 1: ABC TRANSPORTER, PERIPLASMIC BINDING PROTEIN, AMINO ACID

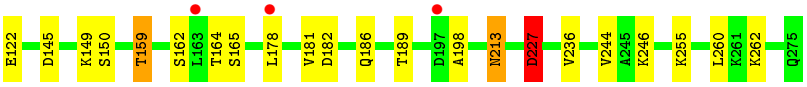
Chain C:



• Molecule 1: ABC TRANSPORTER, PERIPLASMIC BINDING PROTEIN, AMINO ACID

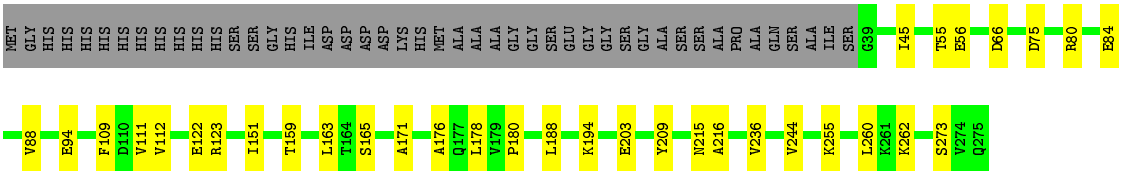
Chain D:





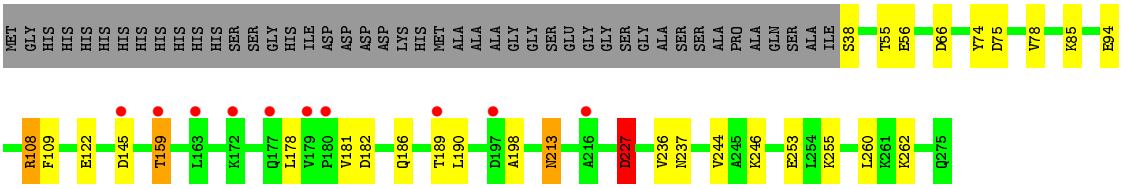
• Molecule 1: ABC TRANSPORTER, PERIPLASMIC BINDING PROTEIN, AMINO ACID

Chain E:



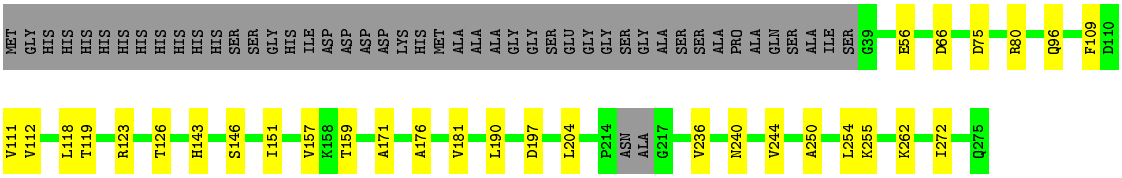
• Molecule 1: ABC TRANSPORTER, PERIPLASMIC BINDING PROTEIN, AMINO ACID

Chain F:



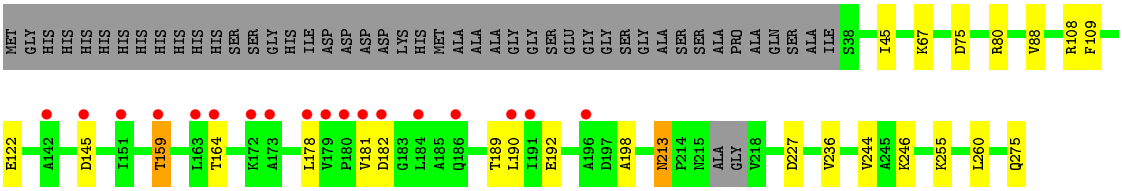
• Molecule 1: ABC TRANSPORTER, PERIPLASMIC BINDING PROTEIN, AMINO ACID

Chain G:



• Molecule 1: ABC TRANSPORTER, PERIPLASMIC BINDING PROTEIN, AMINO ACID

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.09Å 99.83Å 128.83Å 90.00° 91.50° 90.00°	Depositor
Resolution (Å)	48.00 – 2.32 47.98 – 2.32	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.00-2.32) 99.7 (47.98-2.32)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.217 , 0.267 0.215 , 0.261	Depositor DCC
R_{free} test set	4052 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	27.1	Xtriage
Anisotropy	0.725	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 13.9	EDS
Estimated twinning fraction	0.178 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 81031 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14685	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.40 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.8659e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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	0.95	0/1819	0.81	0/2460
1	B	0.86	0/1781	0.94	4/2413 (0.2%)
1	C	0.91	0/1781	0.83	2/2408 (0.1%)
1	D	0.81	0/1789	0.96	5/2421 (0.2%)
1	E	0.97	1/1812 (0.1%)	0.83	1/2449 (0.0%)
1	F	0.80	0/1783	1.01	6/2419 (0.2%)
1	G	0.87	0/1796	0.82	1/2430 (0.0%)
1	H	0.78	0/1749	0.91	4/2371 (0.2%)
All	All	0.87	1/14310 (0.0%)	0.89	23/19371 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	F	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	203	GLU	CG-CD	5.14	1.59	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	108	ARG	NE-CZ-NH2	-25.72	107.44	120.30
1	D	108	ARG	NE-CZ-NH1	-23.20	108.70	120.30
1	B	108	ARG	NE-CZ-NH2	-19.90	110.35	120.30
1	H	108	ARG	NE-CZ-NH2	-18.85	110.87	120.30
1	B	108	ARG	NE-CZ-NH1	16.78	128.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	108	ARG	NE-CZ-NH1	16.32	128.46	120.30
1	H	108	ARG	NE-CZ-NH1	15.78	128.19	120.30
1	D	108	ARG	NE-CZ-NH2	14.90	127.75	120.30
1	D	108	ARG	CD-NE-CZ	13.95	143.13	123.60
1	F	108	ARG	CD-NE-CZ	13.83	142.96	123.60
1	B	108	ARG	CD-NE-CZ	9.31	136.63	123.60
1	H	108	ARG	CD-NE-CZ	9.18	136.45	123.60
1	B	227	ASP	CB-CG-OD2	6.47	124.12	118.30
1	F	108	ARG	CG-CD-NE	-6.36	98.44	111.80
1	D	108	ARG	CG-CD-NE	-6.29	98.60	111.80
1	E	80	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	F	227	ASP	CB-CG-OD2	5.92	123.63	118.30
1	C	80	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	H	80	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	D	227	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	80	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	F	66	ASP	CB-CG-OD1	5.22	123.00	118.30
1	G	80	ARG	NE-CZ-NH1	5.05	122.82	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	108	ARG	Sidechain
1	F	108	ARG	Sidechain

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	1793	0	1772	12	0
1	B	1756	0	1707	27	0
1	C	1756	0	1743	22	0
1	D	1763	0	1745	17	0
1	E	1786	0	1780	19	0
1	F	1757	0	1714	17	0
1	G	1771	0	1739	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1724	0	1667	17	0
2	A	83	0	0	3	0
2	B	60	0	0	2	0
2	C	74	0	0	1	0
2	D	63	0	0	1	0
2	E	85	0	0	1	0
2	F	64	0	0	3	0
2	G	83	0	0	2	0
2	H	67	0	0	2	0
All	All	14685	0	13867	140	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (140) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:VAL:HG22	1:C:111:VAL:CG1	2.02	0.88
1:B:140:LEU:HD21	1:B:154:ILE:HD13	1.55	0.86
1:B:182:ASP:OD1	1:B:186:GLN:HG3	1.76	0.83
1:D:236:VAL:HG21	1:D:244:VAL:HG23	1.61	0.82
1:H:236:VAL:HG21	1:H:244:VAL:HG23	1.63	0.81
1:C:119:THR:HG23	2:C:2031:HOH:O	1.82	0.79
1:F:236[A]:VAL:HG11	1:F:244:VAL:HG23	1.65	0.78
1:B:140:LEU:HD21	1:B:154:ILE:CD1	2.14	0.77
1:C:159:THR:HG21	1:C:171:ALA:HB1	1.68	0.75
1:B:154:ILE:O	1:B:154:ILE:HG23	1.91	0.70
1:G:159:THR:HG21	1:G:171:ALA:HB1	1.75	0.68
1:E:163:LEU:HD21	1:E:180:PRO:HB3	1.76	0.68
1:C:74:TYR:O	1:C:78:VAL:HG23	1.94	0.67
1:B:236:VAL:HG21	1:B:244:VAL:CG2	2.24	0.67
1:F:236[B]:VAL:HG21	1:F:244:VAL:HG23	1.76	0.66
1:G:159:THR:CG2	1:G:176:ALA:HB1	2.26	0.66
1:E:255:LYS:HG3	1:E:260:LEU:HD12	1.77	0.66
1:H:236:VAL:HG21	1:H:244:VAL:CG2	2.27	0.65
1:C:53:VAL:HG13	1:C:111:VAL:HG13	1.79	0.64
2:A:2028:HOH:O	1:B:98[A]:ASP:OD2	2.15	0.63
1:B:154:ILE:O	1:B:154:ILE:CG2	2.45	0.63
1:C:236:VAL:HG21	1:C:244:VAL:CG2	2.28	0.62
1:H:159:THR:HG23	1:H:198:ALA:HB3	1.80	0.62
1:D:236:VAL:HG21	1:D:244:VAL:CG2	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:236[A]:VAL:HG11	1:F:244:VAL:CG2	2.30	0.61
1:A:159:THR:HG21	1:A:171:ALA:HB1	1.81	0.61
1:G:118:LEU:HD12	1:G:123:ARG:HB3	1.84	0.59
1:H:192:GLU:CB	2:H:2051:HOH:O	2.51	0.59
1:B:181:VAL:CG1	1:B:186:GLN:HB2	2.32	0.59
1:F:213:ASN:N	1:F:213:ASN:OD1	2.36	0.59
1:E:163:LEU:CD2	1:E:180:PRO:HB3	2.32	0.58
1:C:53:VAL:HG22	1:C:111:VAL:HG12	1.85	0.58
1:H:213:ASN:OD1	1:H:213:ASN:N	2.36	0.58
1:B:181:VAL:HG21	1:B:190:LEU:HD13	1.85	0.58
1:D:227:ASP:OD1	1:D:227:ASP:N	2.36	0.58
1:E:159:THR:HG21	1:E:176:ALA:CB	2.34	0.57
1:D:213:ASN:N	1:D:213:ASN:OD1	2.38	0.57
1:D:159:THR:HG23	1:D:198:ALA:HB3	1.87	0.57
1:B:181:VAL:HG11	1:B:186:GLN:HB2	1.86	0.57
1:G:255:LYS:NZ	2:G:2038:HOH:O	2.38	0.57
1:C:56:GLU:OE1	1:D:122:GLU:OE2	2.23	0.57
1:C:53:VAL:HG22	1:C:111:VAL:HG11	1.86	0.56
1:B:213:ASN:OD1	1:B:213:ASN:N	2.38	0.56
1:A:216:ALA:HB1	1:A:218:VAL:HG22	1.88	0.56
1:B:159:THR:HG23	1:B:198:ALA:HB3	1.88	0.56
1:C:255:LYS:HG3	1:C:260:LEU:HD12	1.89	0.55
1:B:161:GLN:N	2:B:2042:HOH:O	2.39	0.55
1:G:118:LEU:CD1	1:G:123:ARG:HB3	2.36	0.54
1:F:227:ASP:N	1:F:227:ASP:OD1	2.40	0.54
1:F:159:THR:HG23	1:F:198:ALA:HB3	1.89	0.54
1:A:148:ILE:HG23	1:A:153:ASP:HB2	1.89	0.54
1:E:55:THR:O	1:E:94:GLU:HA	2.08	0.54
1:G:159:THR:HG21	1:G:176:ALA:CB	2.38	0.53
1:B:236:VAL:HG21	1:B:244:VAL:HG22	1.88	0.53
1:G:56:GLU:OE1	1:H:122:GLU:OE2	2.25	0.53
1:G:159:THR:HG22	1:G:176:ALA:HB1	1.90	0.53
1:G:111:VAL:HG22	1:G:236:VAL:HG12	1.89	0.53
1:E:236:VAL:HG21	1:E:244:VAL:CG2	2.39	0.53
1:G:244:VAL:HG11	1:H:164:THR:CG2	2.39	0.52
1:G:157:VAL:HG13	1:G:197:ASP:OD2	2.09	0.52
1:B:181:VAL:HG23	2:B:2042:HOH:O	2.10	0.52
1:D:236:VAL:CG2	1:D:244:VAL:CG2	2.88	0.51
1:F:255:LYS:HG3	1:F:260:LEU:HD12	1.92	0.51
1:E:163:LEU:HD23	2:E:2045:HOH:O	2.10	0.51
1:A:148:ILE:HG23	1:A:153:ASP:CB	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:GLU:OE1	1:B:122:GLU:OE2	2.28	0.51
1:A:244:VAL:HG11	1:B:164:THR:HG22	1.94	0.50
1:H:145:ASP:N	1:H:145:ASP:OD1	2.44	0.50
1:G:240:ASN:O	1:G:244:VAL:HG23	2.12	0.49
1:G:96[B]:GLN:HB2	2:G:2018:HOH:O	2.12	0.49
1:B:255:LYS:HG3	1:B:260:LEU:HD12	1.94	0.49
1:C:244:VAL:HG11	1:D:164:THR:CG2	2.42	0.49
1:G:204:LEU:CD2	1:G:272:ILE:HG21	2.42	0.49
1:E:111:VAL:HG12	1:E:112:VAL:N	2.27	0.49
1:B:140:LEU:CD2	1:B:154:ILE:HD13	2.36	0.49
1:C:122:GLU:OE2	1:D:56:GLU:OE1	2.31	0.49
1:E:159:THR:CG2	1:E:176:ALA:HB1	2.43	0.49
1:D:255:LYS:HG3	1:D:260:LEU:HD12	1.95	0.48
1:A:159:THR:O	1:A:159:THR:CG2	2.61	0.48
1:G:157:VAL:CG1	1:G:197:ASP:HB2	2.44	0.48
1:E:122:GLU:OE2	1:F:56:GLU:OE1	2.32	0.48
1:E:159:THR:O	1:E:159:THR:HG23	2.13	0.48
1:A:39:GLY:N	2:A:2001:HOH:O	2.47	0.48
1:G:111:VAL:HG12	1:G:112:VAL:N	2.29	0.48
1:C:55:THR:O	1:C:94:GLU:HA	2.13	0.48
1:E:45:ILE:HA	1:E:88:VAL:HG11	1.95	0.47
1:A:63:THR:HG23	1:A:63:THR:O	2.14	0.47
1:E:159:THR:HG21	1:E:176:ALA:HB3	1.96	0.47
1:B:145:ASP:OD1	1:B:145:ASP:N	2.47	0.47
1:H:236:VAL:CG2	1:H:244:VAL:CG2	2.93	0.47
1:G:66:ASP:C	1:G:66:ASP:OD1	2.52	0.47
1:B:154:ILE:CG2	1:B:176:ALA:HB2	2.45	0.47
1:F:74:TYR:O	1:F:78:VAL:HG23	2.14	0.46
1:G:181:VAL:CG1	1:G:190:LEU:HD22	2.45	0.46
1:G:244:VAL:HG11	1:H:164:THR:HG22	1.97	0.46
1:B:204:LEU:HD22	1:B:272:ILE:HD13	1.96	0.46
1:E:123:ARG:HD2	2:F:2027:HOH:O	2.16	0.46
1:C:159:THR:CG2	1:C:178:LEU:HD23	2.45	0.46
1:G:159:THR:CG2	1:G:176:ALA:CB	2.94	0.46
1:D:55:THR:O	1:D:94:GLU:HA	2.17	0.46
1:D:145:ASP:OD1	1:D:145:ASP:N	2.48	0.45
1:F:253:GLU:HB3	2:F:2022:HOH:O	2.17	0.45
1:C:179:VAL:CG1	1:C:190:LEU:HD21	2.47	0.45
1:C:244:VAL:HG11	1:D:164:THR:HG22	1.99	0.45
1:E:56:GLU:OE1	1:F:122:GLU:OE2	2.35	0.44
1:E:159:THR:HG21	1:E:176:ALA:HB1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:LEU:HD12	1:E:209:TYR:CE2	2.53	0.44
1:F:145:ASP:OD1	1:F:145:ASP:N	2.50	0.44
1:F:236[A]:VAL:HG13	1:F:237:ASN:O	2.18	0.44
1:C:155:LYS:NZ	1:H:275:GLN:OXT	2.51	0.44
1:A:159:THR:O	1:A:159:THR:HG23	2.18	0.44
1:C:206:VAL:O	1:C:210:LEU:HG	2.17	0.43
1:C:140:LEU:HD13	1:C:200:LEU:CD2	2.47	0.43
1:H:181:VAL:HG21	1:H:190:LEU:HD22	2.00	0.43
1:G:250:ALA:O	1:G:254:LEU:HG	2.18	0.43
1:F:85:LYS:NZ	2:F:2022:HOH:O	2.50	0.43
1:E:255:LYS:HE3	1:E:273:SER:O	2.19	0.43
1:D:65:HIS:NE2	1:D:94:GLU:OE1	2.38	0.43
1:H:67:LYS:HG2	2:H:2014:HOH:O	2.19	0.43
1:C:151:ILE:HD11	1:C:200:LEU:HD21	2.01	0.43
1:B:182:ASP:OD1	1:B:182:ASP:N	2.49	0.43
1:G:190:LEU:HA	1:G:190:LEU:HD12	1.94	0.42
1:E:171:ALA:HB3	1:E:178:LEU:HD21	2.01	0.42
1:D:162:SER:O	1:D:165:SER:OG	2.32	0.42
1:B:186:GLN:H	1:B:186:GLN:CD	2.23	0.42
1:A:122:GLU:OE2	1:B:56:GLU:OE1	2.36	0.42
1:G:244:VAL:HG11	1:H:164:THR:HG21	2.02	0.42
1:C:179:VAL:HG11	1:C:190:LEU:HD21	2.02	0.41
1:H:45:ILE:HA	1:H:88:VAL:HG11	2.02	0.41
1:F:236[A]:VAL:CG1	1:F:244:VAL:CG2	2.99	0.41
1:B:236:VAL:CG2	1:B:244:VAL:CG2	2.97	0.41
1:D:108:ARG:NH1	2:D:2027:HOH:O	2.45	0.41
1:D:181:VAL:CG1	1:D:186:GLN:CB	2.99	0.41
1:H:227:ASP:N	1:H:227:ASP:OD1	2.54	0.41
1:A:169:GLU:HG2	2:A:2053:HOH:O	2.20	0.41
1:F:181:VAL:CG1	1:F:186:GLN:CB	2.99	0.41
1:C:188:LEU:HD23	1:C:188:LEU:HA	1.89	0.41
1:H:255:LYS:HG3	1:H:260:LEU:HD12	2.02	0.41
1:B:236:VAL:CG2	1:B:244:VAL:HG22	2.51	0.41
1:F:55:THR:O	1:F:94:GLU:HA	2.22	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	237/283 (84%)	227 (96%)	9 (4%)	1 (0%)	39 48
1	B	234/283 (83%)	229 (98%)	5 (2%)	0	100 100
1	C	231/283 (82%)	223 (96%)	8 (4%)	0	100 100
1	D	235/283 (83%)	229 (97%)	6 (3%)	0	100 100
1	E	236/283 (83%)	225 (95%)	8 (3%)	3 (1%)	15 14
1	F	237/283 (84%)	232 (98%)	5 (2%)	0	100 100
1	G	234/283 (83%)	226 (97%)	7 (3%)	1 (0%)	39 48
1	H	232/283 (82%)	226 (97%)	6 (3%)	0	100 100
All	All	1876/2264 (83%)	1817 (97%)	54 (3%)	5 (0%)	46 56

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	215	ASN
1	E	216	ALA
1	E	66	ASP
1	G	146	SER
1	A	114	ASN

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	185/221 (84%)	179 (97%)	6 (3%)	46 62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	180/221 (81%)	166 (92%)	14 (8%)	16 19
1	C	182/221 (82%)	177 (97%)	5 (3%)	52 69
1	D	182/221 (82%)	170 (93%)	12 (7%)	21 26
1	E	186/221 (84%)	179 (96%)	7 (4%)	40 54
1	F	179/221 (81%)	167 (93%)	12 (7%)	20 26
1	G	181/221 (82%)	174 (96%)	7 (4%)	39 53
1	H	173/221 (78%)	165 (95%)	8 (5%)	33 44
All	All	1448/1768 (82%)	1377 (95%)	71 (5%)	31 41

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	THR
1	A	75	ASP
1	A	109	PHE
1	A	120	SER
1	A	126	THR
1	A	159	THR
1	B	38	SER
1	B	75	ASP
1	B	109	PHE
1	B	154	ILE
1	B	159	THR
1	B	169	GLU
1	B	178	LEU
1	B	182	ASP
1	B	186	GLN
1	B	189	THR
1	B	190	LEU
1	B	213	ASN
1	B	246	LYS
1	B	270	LYS
1	C	75	ASP
1	C	109	PHE
1	C	123	ARG
1	C	169	GLU
1	C	219	LYS
1	D	75	ASP
1	D	109	PHE
1	D	149	LYS

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Mol	Chain	Res	Type
1	D	150	SER
1	D	159	THR
1	D	178	LEU
1	D	182	ASP
1	D	189	THR
1	D	213	ASN
1	D	227	ASP
1	D	246	LYS
1	D	262	LYS
1	E	75	ASP
1	E	84	GLU
1	E	109	PHE
1	E	151	ILE
1	E	165	SER
1	E	194	LYS
1	E	262	LYS
1	F	38	SER
1	F	75	ASP
1	F	109	PHE
1	F	159	THR
1	F	178	LEU
1	F	182	ASP
1	F	189	THR
1	F	190	LEU
1	F	213	ASN
1	F	227	ASP
1	F	246	LYS
1	F	262	LYS
1	G	75	ASP
1	G	109	PHE
1	G	119	THR
1	G	126	THR
1	G	143	HIS
1	G	151	ILE
1	G	262	LYS
1	H	75	ASP
1	H	109	PHE
1	H	159	THR
1	H	178	LEU
1	H	182	ASP
1	H	189	THR
1	H	213	ASN

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Mol	Chain	Res	Type
1	H	246	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	143	HIS
1	A	144	ASN
1	B	47	ASN
1	D	47	ASN
1	F	47	ASN
1	F	177	GLN
1	H	47	ASN
1	H	144	ASN

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

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	237/283 (83%)	-0.51	0 100 100	12, 25, 43, 56	0
1	B	237/283 (83%)	-0.03	17 (7%) 18 26	14, 25, 155, 190	0
1	C	235/283 (83%)	-0.54	0 100 100	15, 26, 42, 57	1 (0%)
1	D	237/283 (83%)	-0.32	3 (1%) 79 84	15, 26, 67, 75	0
1	E	237/283 (83%)	-0.51	0 100 100	12, 24, 44, 58	0
1	F	238/283 (84%)	-0.18	10 (4%) 40 48	13, 26, 84, 100	0
1	G	235/283 (83%)	-0.45	0 100 100	15, 28, 48, 68	0
1	H	236/283 (83%)	-0.02	18 (7%) 17 24	13, 27, 101, 115	2 (0%)
All	All	1892/2264 (83%)	-0.32	48 (2%) 61 69	12, 26, 86, 190	3 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	163	LEU	5.6
1	H	178	LEU	5.1
1	H	163	LEU	4.7
1	B	180	PRO	4.7
1	B	159	THR	4.1
1	B	178	LEU	4.0
1	B	164	THR	3.9
1	B	190	LEU	3.6
1	H	180	PRO	3.5
1	B	166	ASN	3.5
1	F	197	ASP	3.1
1	H	196	ALA	3.1
1	D	163	LEU	3.1
1	H	184	LEU	3.1
1	F	159	THR	3.1
1	F	180	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	186	GLN	3.0
1	B	168	GLY	3.0
1	D	197	ASP	2.9
1	B	165	SER	2.9
1	B	183	GLY	2.9
1	H	164	THR	2.8
1	H	159	THR	2.8
1	B	177	GLN	2.7
1	H	172	LYS	2.7
1	B	167	TYR	2.6
1	H	181	VAL	2.5
1	F	163	LEU	2.5
1	H	190	LEU	2.5
1	D	178	LEU	2.4
1	F	177	GLN	2.4
1	H	173	ALA	2.4
1	B	172	LYS	2.3
1	B	179	VAL	2.3
1	H	145	ASP	2.3
1	F	179	VAL	2.3
1	H	142	ALA	2.2
1	H	182	ASP	2.2
1	H	151	ILE	2.2
1	F	216	ALA	2.2
1	H	191	ILE	2.1
1	B	197	ASP	2.1
1	F	145	ASP	2.1
1	F	189	THR	2.1
1	H	179	VAL	2.1
1	F	172	LYS	2.0
1	B	152	ALA	2.0
1	B	148	ILE	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.