Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:31 PM GMT

PDB ID	:	1TWY
Title	:	Crystal structure of an ABC-type phosphate transport receptor from Vibrio cholerae
Authors	:	Ramagopal, U.A.; Patskovsky, Y.; Almo, S.C.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2004-07-01
Resolution	:	1.65 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:

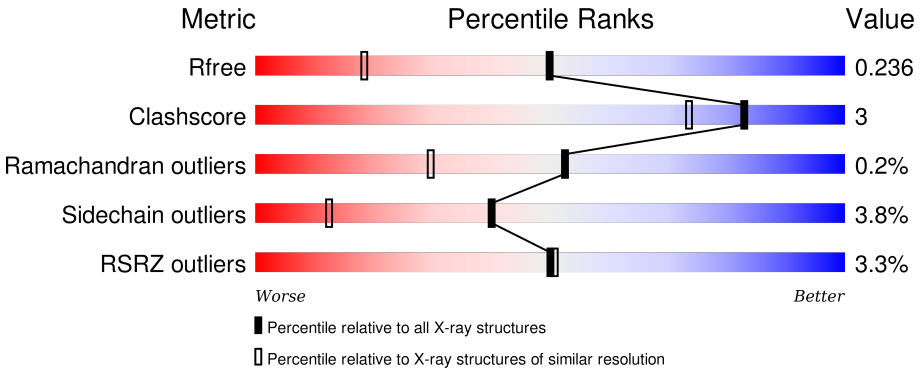
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.65 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	1226 (1.66-1.66)
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (1.66-1.66)

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	290	3% 77% 8% • 14%
1	B	290	3% 75% 9% 16%
1	C	290	3% 71% 12% • 14%
1	D	290	3% 78% 8% 14%
1	E	290	2% 76% 8% • 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	290	2% 72% 11% 15%
1	G	290	4% 74% 11% 14%
1	H	290	2% 73% 11% 14%

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	PO4	C	1507	-	-	X	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16805 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 substrate-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	Se	0	1	0
			1919	1208	324	381	6			
1	B	244	Total	C	N	O	Se	0	2	0
			1890	1191	318	375	6			
1	C	249	Total	C	N	O	Se	0	5	0
			1937	1219	327	385	6			
1	D	249	Total	C	N	O	Se	0	0	0
			1918	1208	324	380	6			
1	E	248	Total	C	N	O	Se	0	2	0
			1917	1207	324	380	6			
1	F	247	Total	C	N	O	Se	0	3	0
			1910	1201	323	380	6			
1	G	249	Total	C	N	O	Se	0	2	0
			1924	1211	324	383	6			
1	H	249	Total	C	N	O	Se	0	5	0
			1937	1219	328	384	6			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	CLONING ARTIFACT	GB 15601562
A	2	SER	-	CLONING ARTIFACT	GB 15601562
A	3	LEU	-	CLONING ARTIFACT	GB 15601562
A	42	MSE	MET	MODIFIED RESIDUE	GB 15601562
A	81	MSE	MET	MODIFIED RESIDUE	GB 15601562
A	163	MSE	MET	MODIFIED RESIDUE	GB 15601562
A	189	MSE	MET	MODIFIED RESIDUE	GB 15601562
A	190	MSE	MET	MODIFIED RESIDUE	GB 15601562
A	275	MSE	MET	MODIFIED RESIDUE	GB 15601562
A	281	GLU	-	CLONING ARTIFACT	GB 15601562
A	282	GLY	-	CLONING ARTIFACT	GB 15601562
A	283	GLY	-	CLONING ARTIFACT	GB 15601562
A	284	SER	-	CLONING ARTIFACT	GB 15601562

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	285	HIS	-	CLONING ARTIFACT	GB 15601562
A	286	HIS	-	CLONING ARTIFACT	GB 15601562
A	287	HIS	-	CLONING ARTIFACT	GB 15601562
A	288	HIS	-	CLONING ARTIFACT	GB 15601562
A	289	HIS	-	CLONING ARTIFACT	GB 15601562
A	290	HIS	-	CLONING ARTIFACT	GB 15601562
B	1	MET	-	CLONING ARTIFACT	GB 15601562
B	2	SER	-	CLONING ARTIFACT	GB 15601562
B	3	LEU	-	CLONING ARTIFACT	GB 15601562
B	42	MSE	MET	MODIFIED RESIDUE	GB 15601562
B	81	MSE	MET	MODIFIED RESIDUE	GB 15601562
B	163	MSE	MET	MODIFIED RESIDUE	GB 15601562
B	189	MSE	MET	MODIFIED RESIDUE	GB 15601562
B	190	MSE	MET	MODIFIED RESIDUE	GB 15601562
B	275	MSE	MET	MODIFIED RESIDUE	GB 15601562
B	281	GLU	-	CLONING ARTIFACT	GB 15601562
B	282	GLY	-	CLONING ARTIFACT	GB 15601562
B	283	GLY	-	CLONING ARTIFACT	GB 15601562
B	284	SER	-	CLONING ARTIFACT	GB 15601562
B	285	HIS	-	CLONING ARTIFACT	GB 15601562
B	286	HIS	-	CLONING ARTIFACT	GB 15601562
B	287	HIS	-	CLONING ARTIFACT	GB 15601562
B	288	HIS	-	CLONING ARTIFACT	GB 15601562
B	289	HIS	-	CLONING ARTIFACT	GB 15601562
B	290	HIS	-	CLONING ARTIFACT	GB 15601562
C	1	MET	-	CLONING ARTIFACT	GB 15601562
C	2	SER	-	CLONING ARTIFACT	GB 15601562
C	3	LEU	-	CLONING ARTIFACT	GB 15601562
C	42	MSE	MET	MODIFIED RESIDUE	GB 15601562
C	81	MSE	MET	MODIFIED RESIDUE	GB 15601562
C	163	MSE	MET	MODIFIED RESIDUE	GB 15601562
C	189	MSE	MET	MODIFIED RESIDUE	GB 15601562
C	190	MSE	MET	MODIFIED RESIDUE	GB 15601562
C	275	MSE	MET	MODIFIED RESIDUE	GB 15601562
C	281	GLU	-	CLONING ARTIFACT	GB 15601562
C	282	GLY	-	CLONING ARTIFACT	GB 15601562
C	283	GLY	-	CLONING ARTIFACT	GB 15601562
C	284	SER	-	CLONING ARTIFACT	GB 15601562
C	285	HIS	-	CLONING ARTIFACT	GB 15601562
C	286	HIS	-	CLONING ARTIFACT	GB 15601562
C	287	HIS	-	CLONING ARTIFACT	GB 15601562
C	288	HIS	-	CLONING ARTIFACT	GB 15601562

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	289	HIS	-	CLONING ARTIFACT	GB 15601562
C	290	HIS	-	CLONING ARTIFACT	GB 15601562
D	1	MET	-	CLONING ARTIFACT	GB 15601562
D	2	SER	-	CLONING ARTIFACT	GB 15601562
D	3	LEU	-	CLONING ARTIFACT	GB 15601562
D	42	MSE	MET	MODIFIED RESIDUE	GB 15601562
D	81	MSE	MET	MODIFIED RESIDUE	GB 15601562
D	163	MSE	MET	MODIFIED RESIDUE	GB 15601562
D	189	MSE	MET	MODIFIED RESIDUE	GB 15601562
D	190	MSE	MET	MODIFIED RESIDUE	GB 15601562
D	275	MSE	MET	MODIFIED RESIDUE	GB 15601562
D	281	GLU	-	CLONING ARTIFACT	GB 15601562
D	282	GLY	-	CLONING ARTIFACT	GB 15601562
D	283	GLY	-	CLONING ARTIFACT	GB 15601562
D	284	SER	-	CLONING ARTIFACT	GB 15601562
D	285	HIS	-	CLONING ARTIFACT	GB 15601562
D	286	HIS	-	CLONING ARTIFACT	GB 15601562
D	287	HIS	-	CLONING ARTIFACT	GB 15601562
D	288	HIS	-	CLONING ARTIFACT	GB 15601562
D	289	HIS	-	CLONING ARTIFACT	GB 15601562
D	290	HIS	-	CLONING ARTIFACT	GB 15601562
E	1	MET	-	CLONING ARTIFACT	GB 15601562
E	2	SER	-	CLONING ARTIFACT	GB 15601562
E	3	LEU	-	CLONING ARTIFACT	GB 15601562
E	42	MSE	MET	MODIFIED RESIDUE	GB 15601562
E	81	MSE	MET	MODIFIED RESIDUE	GB 15601562
E	163	MSE	MET	MODIFIED RESIDUE	GB 15601562
E	189	MSE	MET	MODIFIED RESIDUE	GB 15601562
E	190	MSE	MET	MODIFIED RESIDUE	GB 15601562
E	275	MSE	MET	MODIFIED RESIDUE	GB 15601562
E	281	GLU	-	CLONING ARTIFACT	GB 15601562
E	282	GLY	-	CLONING ARTIFACT	GB 15601562
E	283	GLY	-	CLONING ARTIFACT	GB 15601562
E	284	SER	-	CLONING ARTIFACT	GB 15601562
E	285	HIS	-	CLONING ARTIFACT	GB 15601562
E	286	HIS	-	CLONING ARTIFACT	GB 15601562
E	287	HIS	-	CLONING ARTIFACT	GB 15601562
E	288	HIS	-	CLONING ARTIFACT	GB 15601562
E	289	HIS	-	CLONING ARTIFACT	GB 15601562
E	290	HIS	-	CLONING ARTIFACT	GB 15601562
F	1	MET	-	CLONING ARTIFACT	GB 15601562
F	2	SER	-	CLONING ARTIFACT	GB 15601562

Continued on next page...

Continued from previous page...

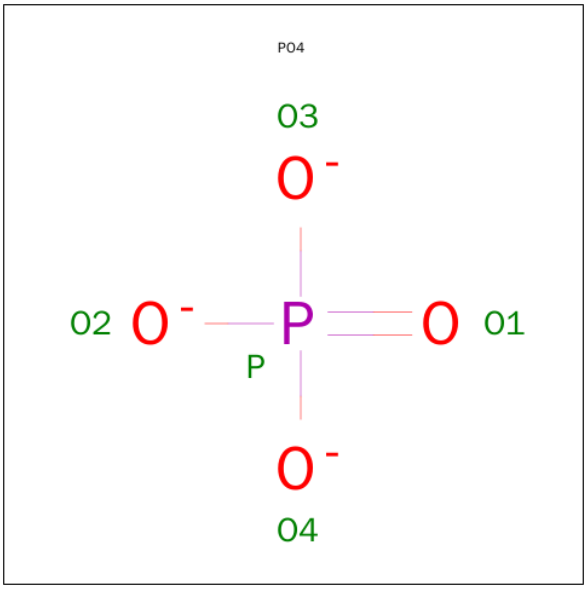
Chain	Residue	Modelled	Actual	Comment	Reference
F	3	LEU	-	CLONING ARTIFACT	GB 15601562
F	42	MSE	MET	MODIFIED RESIDUE	GB 15601562
F	81	MSE	MET	MODIFIED RESIDUE	GB 15601562
F	163	MSE	MET	MODIFIED RESIDUE	GB 15601562
F	189	MSE	MET	MODIFIED RESIDUE	GB 15601562
F	190	MSE	MET	MODIFIED RESIDUE	GB 15601562
F	275	MSE	MET	MODIFIED RESIDUE	GB 15601562
F	281	GLU	-	CLONING ARTIFACT	GB 15601562
F	282	GLY	-	CLONING ARTIFACT	GB 15601562
F	283	GLY	-	CLONING ARTIFACT	GB 15601562
F	284	SER	-	CLONING ARTIFACT	GB 15601562
F	285	HIS	-	CLONING ARTIFACT	GB 15601562
F	286	HIS	-	CLONING ARTIFACT	GB 15601562
F	287	HIS	-	CLONING ARTIFACT	GB 15601562
F	288	HIS	-	CLONING ARTIFACT	GB 15601562
F	289	HIS	-	CLONING ARTIFACT	GB 15601562
F	290	HIS	-	CLONING ARTIFACT	GB 15601562
G	1	MET	-	CLONING ARTIFACT	GB 15601562
G	2	SER	-	CLONING ARTIFACT	GB 15601562
G	3	LEU	-	CLONING ARTIFACT	GB 15601562
G	42	MSE	MET	MODIFIED RESIDUE	GB 15601562
G	81	MSE	MET	MODIFIED RESIDUE	GB 15601562
G	163	MSE	MET	MODIFIED RESIDUE	GB 15601562
G	189	MSE	MET	MODIFIED RESIDUE	GB 15601562
G	190	MSE	MET	MODIFIED RESIDUE	GB 15601562
G	275	MSE	MET	MODIFIED RESIDUE	GB 15601562
G	281	GLU	-	CLONING ARTIFACT	GB 15601562
G	282	GLY	-	CLONING ARTIFACT	GB 15601562
G	283	GLY	-	CLONING ARTIFACT	GB 15601562
G	284	SER	-	CLONING ARTIFACT	GB 15601562
G	285	HIS	-	CLONING ARTIFACT	GB 15601562
G	286	HIS	-	CLONING ARTIFACT	GB 15601562
G	287	HIS	-	CLONING ARTIFACT	GB 15601562
G	288	HIS	-	CLONING ARTIFACT	GB 15601562
G	289	HIS	-	CLONING ARTIFACT	GB 15601562
G	290	HIS	-	CLONING ARTIFACT	GB 15601562
H	1	MET	-	CLONING ARTIFACT	GB 15601562
H	2	SER	-	CLONING ARTIFACT	GB 15601562
H	3	LEU	-	CLONING ARTIFACT	GB 15601562
H	42	MSE	MET	MODIFIED RESIDUE	GB 15601562
H	81	MSE	MET	MODIFIED RESIDUE	GB 15601562
H	163	MSE	MET	MODIFIED RESIDUE	GB 15601562

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	189	MSE	MET	MODIFIED RESIDUE	GB 15601562
H	190	MSE	MET	MODIFIED RESIDUE	GB 15601562
H	275	MSE	MET	MODIFIED RESIDUE	GB 15601562
H	281	GLU	-	CLONING ARTIFACT	GB 15601562
H	282	GLY	-	CLONING ARTIFACT	GB 15601562
H	283	GLY	-	CLONING ARTIFACT	GB 15601562
H	284	SER	-	CLONING ARTIFACT	GB 15601562
H	285	HIS	-	CLONING ARTIFACT	GB 15601562
H	286	HIS	-	CLONING ARTIFACT	GB 15601562
H	287	HIS	-	CLONING ARTIFACT	GB 15601562
H	288	HIS	-	CLONING ARTIFACT	GB 15601562
H	289	HIS	-	CLONING ARTIFACT	GB 15601562
H	290	HIS	-	CLONING ARTIFACT	GB 15601562

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total O P 5 4 1	0	0
2	H	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is water.

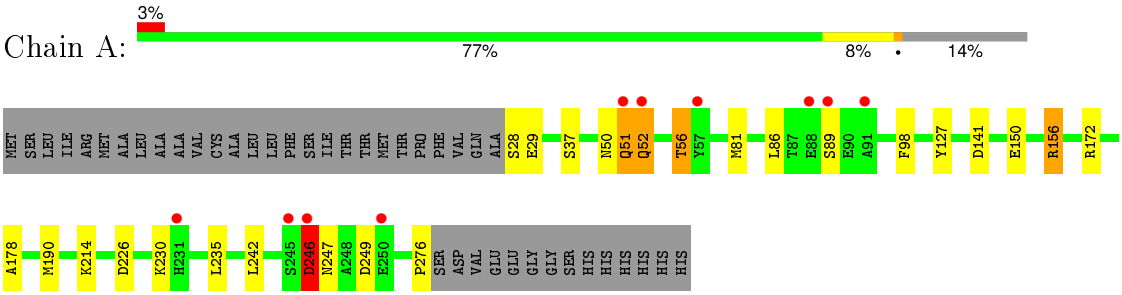
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	177	Total O 177 177	0	0
4	B	190	Total O 190 190	0	0
4	C	159	Total O 159 159	0	0
4	D	145	Total O 145 145	0	0
4	E	160	Total O 160 160	0	0
4	F	216	Total O 216 216	0	0
4	G	163	Total O 163 163	0	0
4	H	202	Total O 202 202	0	0

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.

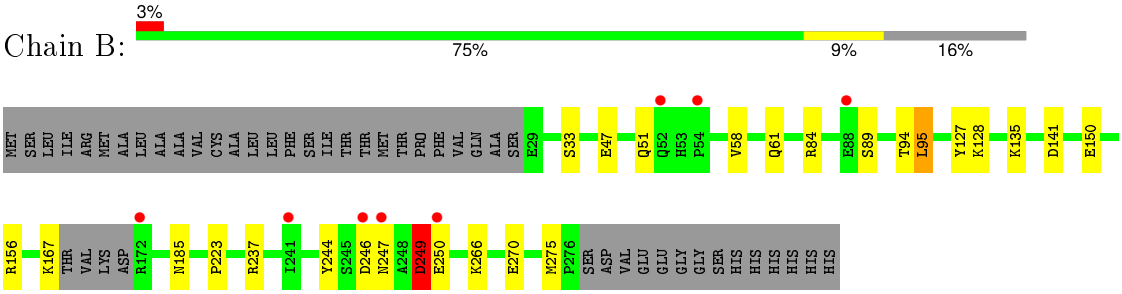
- Molecule 1: ABC transporter, periplasmic substrate-binding protein

Chain A:



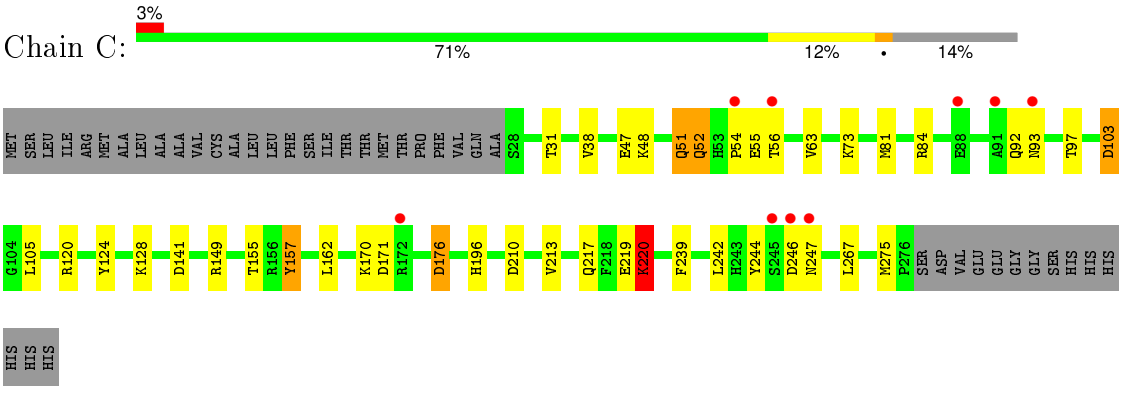
- Molecule 1: ABC transporter, periplasmic substrate-binding protein

Chain B:



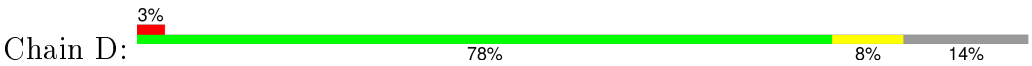
- Molecule 1: ABC transporter, periplasmic substrate-binding protein

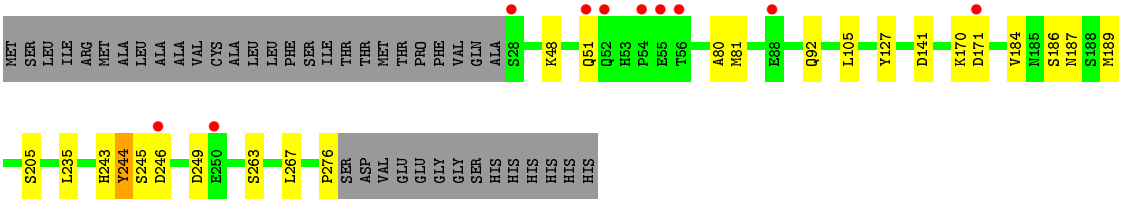
Chain C:



- Molecule 1: ABC transporter, periplasmic substrate-binding protein

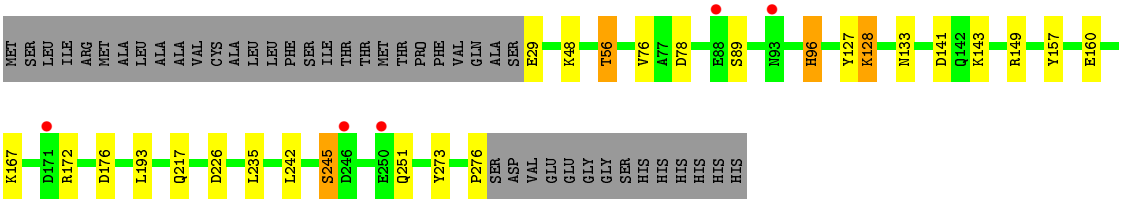
Chain D:





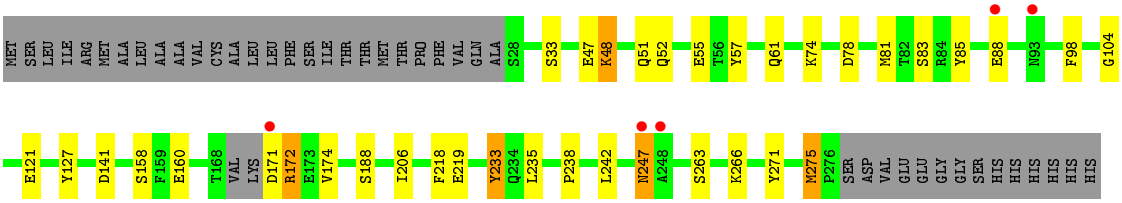
• Molecule 1: ABC transporter, periplasmic substrate-binding protein

Chain E:



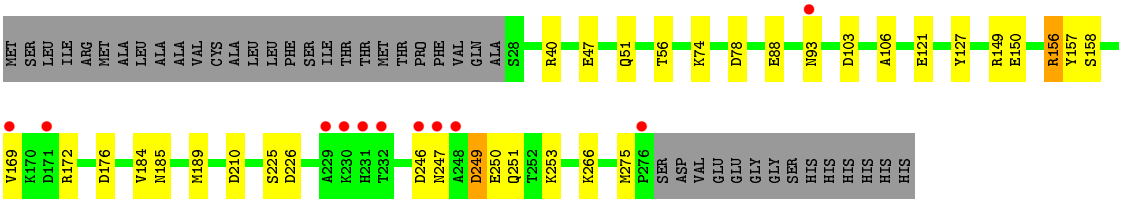
• Molecule 1: ABC transporter, periplasmic substrate-binding protein

Chain F:



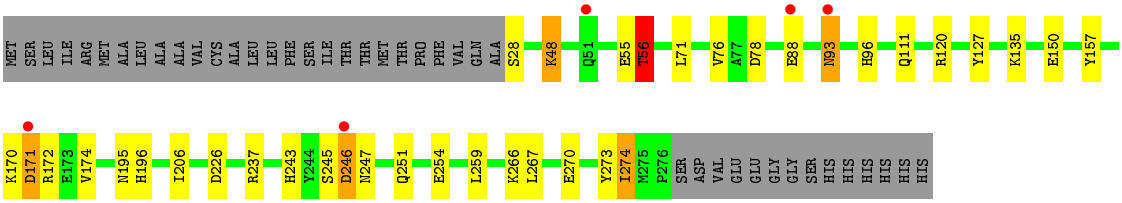
• Molecule 1: ABC transporter, periplasmic substrate-binding protein

Chain G:



• Molecule 1: ABC transporter, periplasmic substrate-binding protein

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	84.63Å 103.93Å 126.69Å 90.00° 102.35° 90.00°	Depositor
Resolution (Å)	19.73 – 1.65 24.84 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.73-1.65) 99.7 (24.84-1.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.193 , 0.231 0.202 , 0.236	Depositor DCC
R_{free} test set	7738 reflections (3.12%)	DCC
Wilson B-factor (Å^2)	20.8	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	1 of 255867 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16805	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: PO4, MG

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	1.32	6/1947 (0.3%)	1.18	9/2626 (0.3%)
1	B	1.36	3/1922 (0.2%)	1.19	7/2592 (0.3%)
1	C	1.37	6/1982 (0.3%)	1.25	14/2674 (0.5%)
1	D	1.26	5/1942 (0.3%)	1.14	5/2621 (0.2%)
1	E	1.31	4/1949 (0.2%)	1.22	8/2629 (0.3%)
1	F	1.38	15/1947 (0.8%)	1.22	7/2625 (0.3%)
1	G	1.31	7/1956 (0.4%)	1.22	12/2638 (0.5%)
1	H	1.36	3/1984 (0.2%)	1.24	10/2676 (0.4%)
All	All	1.33	49/15629 (0.3%)	1.21	72/21081 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	G	0	1
All	All	0	2

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	121	GLU	CD-OE1	9.52	1.36	1.25
1	G	121	GLU	CD-OE1	9.17	1.35	1.25
1	B	275	MSE	SE-CE	-7.96	1.48	1.95
1	F	174	VAL	CB-CG2	-7.59	1.36	1.52
1	F	55	GLU	CD-OE2	7.32	1.33	1.25
1	F	121	GLU	CG-CD	6.95	1.62	1.51
1	C	213	VAL	CB-CG2	-6.89	1.38	1.52
1	D	127	TYR	CE2-CZ	-6.86	1.29	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	TYR	CE2-CZ	-6.82	1.29	1.38
1	G	121	GLU	CG-CD	6.67	1.61	1.51
1	C	219	GLU	CD-OE2	-6.58	1.18	1.25
1	E	157	TYR	CD2-CE2	6.45	1.49	1.39
1	A	37	SER	CB-OG	6.38	1.50	1.42
1	G	106	ALA	CA-CB	-6.31	1.39	1.52
1	C	244	TYR	CE1-CZ	6.28	1.46	1.38
1	G	127	TYR	CD2-CE2	-6.26	1.29	1.39
1	B	58	VAL	CB-CG1	6.24	1.66	1.52
1	G	158	SER	CB-OG	-6.21	1.34	1.42
1	H	157	TYR	CG-CD2	-6.05	1.31	1.39
1	C	124	TYR	CD1-CE1	-6.03	1.30	1.39
1	D	81	MSE	CB-CG	-5.96	1.34	1.52
1	E	273	TYR	CG-CD2	-5.95	1.31	1.39
1	H	174	VAL	CB-CG1	-5.78	1.40	1.52
1	E	160	GLU	CD-OE1	-5.70	1.19	1.25
1	C	157	TYR	CD1-CE1	5.69	1.47	1.39
1	F	275	MSE	SE-CE	-5.69	1.61	1.95
1	C	157	TYR	CB-CG	5.61	1.60	1.51
1	D	244	TYR	CB-CG	-5.54	1.43	1.51
1	F	188[A]	SER	N-CA	-5.54	1.35	1.46
1	F	188[B]	SER	N-CA	-5.54	1.35	1.46
1	G	157	TYR	CB-CG	-5.43	1.43	1.51
1	H	48	LYS	CD-CE	5.42	1.64	1.51
1	B	237	ARG	NE-CZ	5.38	1.40	1.33
1	F	158[A]	SER	CB-OG	-5.36	1.35	1.42
1	F	158[B]	SER	CB-OG	-5.36	1.35	1.42
1	A	98	PHE	CE2-CZ	-5.36	1.27	1.37
1	F	233	TYR	CE2-CZ	-5.36	1.31	1.38
1	F	85	TYR	CD1-CE1	-5.35	1.31	1.39
1	F	81	MSE	CB-CG	-5.29	1.36	1.52
1	A	150	GLU	CD-OE2	5.25	1.31	1.25
1	E	217	GLN	CG-CD	5.23	1.63	1.51
1	F	218	PHE	CE2-CZ	5.22	1.47	1.37
1	F	219	GLU	CD-OE2	-5.13	1.20	1.25
1	D	186	SER	CA-CB	5.07	1.60	1.52
1	D	80	ALA	CA-CB	-5.07	1.41	1.52
1	G	47	GLU	CD-OE1	5.05	1.31	1.25
1	A	190	MSE	SE-CE	-5.03	1.65	1.95
1	A	214	LYS	CE-NZ	5.03	1.61	1.49
1	F	271	TYR	CD2-CE2	-5.02	1.31	1.39

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	156	ARG	NE-CZ-NH1	10.78	125.69	120.30
1	E	276	PRO	CA-C-O	-9.72	96.88	120.20
1	G	156	ARG	NE-CZ-NH2	-9.58	115.51	120.30
1	G	156	ARG	NE-CZ-NH1	9.51	125.06	120.30
1	A	156	ARG	NE-CZ-NH2	-9.46	115.57	120.30
1	E	78	ASP	CB-CG-OD2	8.79	126.22	118.30
1	B	141	ASP	CB-CG-OD1	8.74	126.17	118.30
1	H	78	ASP	CB-CG-OD2	8.74	126.17	118.30
1	E	226	ASP	CB-CG-OD2	8.44	125.90	118.30
1	F	141	ASP	CB-CG-OD1	8.09	125.58	118.30
1	C	81	MSE	CG-SE-CE	-8.04	81.20	98.90
1	B	237	ARG	NE-CZ-NH1	-7.87	116.37	120.30
1	D	141	ASP	CB-CG-OD2	7.69	125.22	118.30
1	H	78	ASP	CB-CG-OD1	-7.30	111.73	118.30
1	G	172	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	A	141	ASP	CB-CG-OD1	7.09	124.68	118.30
1	B	246	ASP	CB-CG-OD1	7.08	124.67	118.30
1	G	78	ASP	CB-CG-OD2	7.05	124.64	118.30
1	B	84	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	E	141	ASP	CB-CG-OD2	6.96	124.56	118.30
1	C	220	LYS	CD-CE-NZ	6.93	127.64	111.70
1	E	149	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	81	MSE	CG-SE-CE	-6.79	83.97	98.90
1	A	276	PRO	CA-C-O	-6.75	104.00	120.20
1	D	276	PRO	CA-C-O	-6.68	104.18	120.20
1	H	127	TYR	CB-CG-CD2	-6.65	117.01	121.00
1	D	235	LEU	CB-CG-CD2	6.62	122.26	111.00
1	C	84	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	G	226	ASP	CB-CG-OD2	6.47	124.12	118.30
1	F	98	PHE	CB-CG-CD1	-6.45	116.29	120.80
1	D	171	ASP	CB-CG-OD2	6.33	124.00	118.30
1	H	237	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	F	242	LEU	CA-CB-CG	6.32	129.84	115.30
1	B	249	ASP	CB-CG-OD2	6.24	123.92	118.30
1	F	160	GLU	OE1-CD-OE2	6.21	130.76	123.30
1	C	63	VAL	CG1-CB-CG2	6.13	120.71	110.90
1	G	103	ASP	CB-CG-OD2	6.01	123.70	118.30
1	C	176	ASP	CB-CG-OD2	6.00	123.70	118.30
1	C	141	ASP	CB-CG-OD1	5.97	123.67	118.30
1	H	150	GLU	OE1-CD-OE2	-5.93	116.18	123.30
1	C	149	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	235	LEU	CB-CG-CD2	5.86	120.97	111.00
1	H	226	ASP	CB-CG-OD2	5.85	123.56	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	78	ASP	CB-CG-OD2	5.84	123.56	118.30
1	C	103[A]	ASP	CB-CG-OD2	5.82	123.54	118.30
1	C	103[B]	ASP	CB-CG-OD2	5.82	123.54	118.30
1	C	246	ASP	CB-CG-OD2	5.72	123.45	118.30
1	C	171	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	135	LYS	CD-CE-NZ	5.65	124.70	111.70
1	H	56	THR	OG1-CB-CG2	-5.63	97.05	110.00
1	G	40	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	E	193	LEU	CB-CG-CD1	5.49	120.33	111.00
1	E	127	TYR	CZ-CE2-CD2	5.47	124.72	119.80
1	A	246	ASP	CB-CG-OD2	5.41	123.17	118.30
1	F	98	PHE	CB-CG-CD2	5.37	124.56	120.80
1	G	176	ASP	CB-CG-OD1	-5.37	113.47	118.30
1	C	210	ASP	CB-CG-OD2	5.33	123.10	118.30
1	H	71	LEU	CB-CG-CD2	5.32	120.04	111.00
1	E	235	LEU	CB-CG-CD2	5.30	120.02	111.00
1	G	210	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	H	274	ILE	CG1-CB-CG2	-5.29	99.75	111.40
1	C	157	TYR	CB-CG-CD1	5.22	124.13	121.00
1	G	149	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	226	ASP	CB-CG-OD2	5.12	122.91	118.30
1	H	259	LEU	CB-CG-CD1	-5.10	102.34	111.00
1	D	249	ASP	CB-CG-OD2	5.08	122.87	118.30
1	C	157	TYR	CA-CB-CG	5.07	123.04	113.40
1	G	121	GLU	CG-CD-OE1	5.06	128.43	118.30
1	G	249	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	249	ASP	CB-CG-OD2	5.03	122.83	118.30
1	F	127	TYR	CB-CG-CD1	5.03	124.02	121.00
1	B	127	TYR	CB-CG-CD1	5.02	124.01	121.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	196	HIS	Sidechain
1	G	246	ASP	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	1919	0	1927	7	0
1	B	1890	0	1891	8	0
1	C	1937	0	1937	23	0
1	D	1918	0	1926	10	0
1	E	1917	0	1924	12	0
1	F	1910	0	1908	14	0
1	G	1924	0	1929	7	0
1	H	1937	0	1950	20	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	2	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
3	A	1	0	0	0	0
4	A	177	0	0	3	0
4	B	190	0	0	4	0
4	C	159	0	0	7	0
4	D	145	0	0	4	0
4	E	160	0	0	1	0
4	F	216	0	0	5	0
4	G	163	0	0	2	0
4	H	202	0	0	7	0
All	All	16805	0	15392	95	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 3.

All (95) 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:103[B]:ASP:OD1	4:C:1560:HOH:O	1.57	1.15
2:C:1507:PO4:O3	4:C:1666:HOH:O	1.75	1.05
1:H:266[B]:LYS:HD2	4:H:1568:HOH:O	1.55	1.04
1:B:61:GLN:HG3	4:B:1686:HOH:O	1.69	0.91
1:C:31:THR:HG23	4:C:1647:HOH:O	1.75	0.85
1:H:254[A]:GLU:OE1	4:H:1696:HOH:O	1.92	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:TYR:CE1	4:F:1717:HOH:O	2.38	0.75
1:A:246:ASP:OD1	1:A:247:ASN:N	2.22	0.72
1:H:246:ASP:HB2	1:H:247:ASN:ND2	2.07	0.70
1:C:217:GLN:OE1	1:C:220:LYS:HE2	1.91	0.70
1:G:275:MSE:HE2	1:G:275:MSE:HA	1.78	0.66
1:H:48:LYS:HD2	1:H:267:LEU:HD11	1.77	0.66
1:C:120:ARG:NH2	1:C:162:LEU:O	2.28	0.66
1:C:128:LYS:NZ	1:C:176:ASP:OD2	2.24	0.66
1:C:217:GLN:OE1	1:C:220:LYS:CE	2.44	0.65
1:B:95:LEU:CD1	1:B:244:TYR:CE1	2.82	0.62
1:E:56:THR:HG22	4:E:1652:HOH:O	2.00	0.62
1:D:170:LYS:NZ	4:D:1619:HOH:O	2.31	0.62
1:C:73:LYS:HE2	1:C:92:GLN:HE21	1.64	0.61
1:E:172:ARG:HD2	4:F:1717:HOH:O	2.01	0.61
1:E:29:GLU:OE2	1:F:172:ARG:NH2	2.35	0.60
1:C:220:LYS:HA	1:C:220:LYS:HE2	1.84	0.59
1:C:97:THR:HG22	1:C:242:LEU:HD23	1.85	0.59
1:C:54:PRO:O	1:D:170:LYS:HD2	2.04	0.58
1:A:50:ASN:ND2	1:A:56:THR:O	2.37	0.57
1:G:156:ARG:NE	4:G:1634:HOH:O	2.37	0.57
1:D:105:LEU:CD2	4:D:1559:HOH:O	2.54	0.56
1:D:105:LEU:HD23	4:D:1559:HOH:O	2.06	0.55
1:C:157:TYR:HB3	4:C:1620:HOH:O	2.06	0.55
1:C:220:LYS:HD3	4:C:1661:HOH:O	2.07	0.54
1:E:29:GLU:N	1:E:251:GLN:HE22	2.05	0.54
1:E:133:ASN:HD22	1:E:143:LYS:NZ	2.06	0.54
1:F:104:GLY:HA3	1:F:206:ILE:HD12	1.89	0.54
1:C:55:GLU:HG2	1:C:56:THR:CG2	2.39	0.53
1:H:120:ARG:HD3	4:H:1694:HOH:O	2.09	0.53
1:F:48:LYS:NZ	1:F:52:GLN:HE22	2.07	0.52
1:E:128:LYS:HE3	1:E:176:ASP:OD2	2.09	0.52
1:H:273:TYR:C	1:H:274:ILE:HD12	2.30	0.52
1:C:51:GLN:HB3	1:C:52:GLN:HE21	1.75	0.52
1:H:274:ILE:HD12	1:H:274:ILE:N	2.26	0.51
1:C:275:MSE:HA	1:C:275:MSE:HE2	1.93	0.50
1:A:178:ALA:HB3	4:A:1578:HOH:O	2.11	0.50
1:D:184:VAL:HG12	1:D:189:MSE:HE2	1.94	0.50
1:G:56:THR:HB	1:G:251:GLN:NE2	2.27	0.50
1:D:92:GLN:NE2	1:D:244:TYR:OH	2.43	0.49
1:H:266[A]:LYS:NZ	1:H:270:GLU:OE1	2.41	0.49
2:C:1507:PO4:P	4:C:1666:HOH:O	2.61	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:LYS:HD2	1:C:267:LEU:HD11	1.96	0.47
1:C:54:PRO:O	1:D:170:LYS:CD	2.62	0.47
1:D:243:HIS:ND1	4:D:1626:HOH:O	2.35	0.47
1:B:156:ARG:NE	4:B:1665:HOH:O	2.48	0.47
1:B:33:SER:OG	1:B:61:GLN:NE2	2.48	0.46
1:G:74:LYS:HD3	1:H:76:VAL:HG11	1.97	0.46
1:A:156:ARG:NE	4:A:1586:HOH:O	2.48	0.46
1:G:150:GLU:OE1	1:G:185:ASN:HA	2.16	0.46
1:F:57:TYR:CZ	4:F:1717:HOH:O	2.67	0.45
1:B:244:TYR:OH	1:D:246:ASP:HB3	2.16	0.45
1:G:251:GLN:HG3	4:G:1657:HOH:O	2.17	0.45
1:A:86:LEU:HD11	1:A:242:LEU:HD21	1.98	0.45
1:C:157:TYR:CB	4:C:1620:HOH:O	2.65	0.45
1:D:187:ASN:HD21	1:D:205:SER:H	1.65	0.45
1:E:76:VAL:HG11	1:F:74:LYS:HD3	1.99	0.44
1:C:55:GLU:HG2	1:C:56:THR:HG22	2.00	0.44
1:F:48:LYS:HZ2	1:F:52:GLN:HE22	1.65	0.44
1:B:156:ARG:CZ	4:B:1665:HOH:O	2.66	0.44
1:E:76:VAL:HG11	1:F:74:LYS:CE	2.47	0.44
1:H:56:THR:HG21	4:H:1642:HOH:O	2.18	0.43
1:E:242:LEU:N	1:E:242:LEU:HD23	2.33	0.43
1:H:243:HIS:CE1	1:H:245:SER:HB3	2.54	0.43
1:H:245:SER:O	1:H:246:ASP:C	2.51	0.43
1:C:105:LEU:HD21	1:C:155:THR:HG23	1.99	0.43
1:H:266[B]:LYS:CD	4:H:1568:HOH:O	2.36	0.42
1:C:55:GLU:HG2	1:C:56:THR:HG23	2.01	0.42
1:H:195:ASN:OD1	1:H:196:HIS:CE1	2.73	0.42
1:F:57:TYR:CD1	4:F:1717:HOH:O	2.67	0.42
1:F:275:MSE:HE2	1:F:275:MSE:HA	2.00	0.42
1:H:55:GLU:HG2	1:H:56:THR:HG22	2.01	0.42
1:H:170:LYS:O	1:H:171:ASP:CB	2.67	0.42
1:G:184:VAL:HG12	1:G:189:MSE:HE2	2.02	0.42
1:E:96:HIS:CD2	1:E:245:SER:OG	2.73	0.42
1:H:111:GLN:HB2	4:H:1707:HOH:O	2.19	0.42
1:A:156:ARG:CZ	4:A:1586:HOH:O	2.68	0.41
1:F:233:TYR:CE2	1:F:235:LEU:HB2	2.56	0.41
1:C:170:LYS:HD3	1:C:170:LYS:HA	1.93	0.41
1:H:251:GLN:HG2	4:H:1696:HOH:O	2.21	0.41
1:E:128:LYS:CE	1:E:176:ASP:OD2	2.67	0.41
1:A:51:GLN:HG2	1:A:52:GLN:N	2.35	0.41
1:F:33:SER:OG	1:F:61:GLN:NE2	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:ARG:CD	4:F:1717:HOH:O	2.67	0.40
1:B:150:GLU:OE1	1:B:185:ASN:HA	2.21	0.40
1:C:38:VAL:HG22	1:C:239:PHE:CG	2.56	0.40
1:F:83:SER:HA	1:F:238:PRO:O	2.21	0.40
1:H:93:ASN:HA	1:H:93:ASN:HD22	1.77	0.40
1:B:223:PRO:HD2	4:B:1688:HOH:O	2.20	0.40
1:F:247:ASN:HD22	1:H:96:HIS:HE1	1.70	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	248/290 (86%)	242 (98%)	6 (2%)	0	100	100
1	B	242/290 (83%)	238 (98%)	3 (1%)	1 (0%)	39	18
1	C	252/290 (87%)	245 (97%)	7 (3%)	0	100	100
1	D	247/290 (85%)	243 (98%)	4 (2%)	0	100	100
1	E	248/290 (86%)	239 (96%)	8 (3%)	1 (0%)	39	18
1	F	246/290 (85%)	241 (98%)	4 (2%)	1 (0%)	39	18
1	G	249/290 (86%)	243 (98%)	6 (2%)	0	100	100
1	H	252/290 (87%)	249 (99%)	3 (1%)	0	100	100
All	All	1984/2320 (86%)	1940 (98%)	41 (2%)	3 (0%)	52	30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	245	SER
1	F	172	ARG
1	B	249	ASP

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	214/241 (89%)	205 (96%)	9 (4%)	36 10
1	B	210/241 (87%)	197 (94%)	13 (6%)	23 4
1	C	218/241 (90%)	212 (97%)	6 (3%)	51 21
1	D	213/241 (88%)	208 (98%)	5 (2%)	58 30
1	E	214/241 (89%)	208 (97%)	6 (3%)	51 21
1	F	214/241 (89%)	206 (96%)	8 (4%)	41 13
1	G	215/241 (89%)	205 (95%)	10 (5%)	32 8
1	H	218/241 (90%)	208 (95%)	10 (5%)	33 8
All	All	1716/1928 (89%)	1649 (96%)	67 (4%)	40 12

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	29	GLU
1	A	51	GLN
1	A	52	GLN
1	A	56	THR
1	A	89	SER
1	A	172	ARG
1	A	230	LYS
1	A	246	ASP
1	B	47	GLU
1	B	51	GLN
1	B	89	SER
1	B	94	THR
1	B	95	LEU
1	B	128	LYS
1	B	167	LYS
1	B	247	ASN
1	B	249	ASP
1	B	250	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	266	LYS
1	B	270[A]	GLU
1	B	270[B]	GLU
1	C	47	GLU
1	C	51	GLN
1	C	52	GLN
1	C	93	ASN
1	C	220	LYS
1	C	247	ASN
1	D	48	LYS
1	D	51	GLN
1	D	245	SER
1	D	263	SER
1	D	267	LEU
1	E	48	LYS
1	E	56	THR
1	E	89	SER
1	E	96	HIS
1	E	128	LYS
1	E	167	LYS
1	F	47	GLU
1	F	48	LYS
1	F	51	GLN
1	F	88	GLU
1	F	171	ASP
1	F	247	ASN
1	F	263	SER
1	F	266	LYS
1	G	51	GLN
1	G	88	GLU
1	G	93	ASN
1	G	169	VAL
1	G	225	SER
1	G	247	ASN
1	G	249	ASP
1	G	250	GLU
1	G	253	LYS
1	G	266	LYS
1	H	28	SER
1	H	56	THR
1	H	88	GLU
1	H	93	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	135	LYS
1	H	171	ASP
1	H	172[A]	ARG
1	H	172[B]	ARG
1	H	206	ILE
1	H	246	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	61	GLN
1	A	93	ASN
1	A	196	HIS
1	A	231	HIS
1	B	61	GLN
1	B	140	ASN
1	B	196	HIS
1	C	52	GLN
1	C	92	GLN
1	C	187	ASN
1	C	251	GLN
1	D	61	GLN
1	D	92	GLN
1	D	130	GLN
1	D	187	ASN
1	D	196	HIS
1	E	51	GLN
1	E	61	GLN
1	E	92	GLN
1	E	96	HIS
1	E	196	HIS
1	F	52	GLN
1	F	61	GLN
1	F	196	HIS
1	G	52	GLN
1	G	142	GLN
1	G	247	ASN
1	G	251	GLN
1	H	93	ASN
1	H	96	HIS
1	H	231	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

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

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	PO4	A	1500	-	4,4,4	1.58	1 (25%)	6,6,6	0.27	0
2	PO4	B	1501	-	4,4,4	0.73	0	6,6,6	0.25	0
2	PO4	C	1507	-	4,4,4	0.65	0	6,6,6	0.30	0
2	PO4	D	1502	-	4,4,4	0.89	0	6,6,6	0.29	0
2	PO4	E	1503	-	4,4,4	1.62	1 (25%)	6,6,6	0.31	0
2	PO4	F	1504	-	4,4,4	1.14	0	6,6,6	0.33	0
2	PO4	G	1505	-	4,4,4	1.06	0	6,6,6	0.30	0
2	PO4	H	1506	-	4,4,4	1.15	0	6,6,6	0.31	0

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	PO4	A	1500	-	-	0/0/0/0	0/0/0/0
2	PO4	B	1501	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	C	1507	-	-	0/0/0/0	0/0/0/0
2	PO4	D	1502	-	-	0/0/0/0	0/0/0/0
2	PO4	E	1503	-	-	0/0/0/0	0/0/0/0
2	PO4	F	1504	-	-	0/0/0/0	0/0/0/0
2	PO4	G	1505	-	-	0/0/0/0	0/0/0/0
2	PO4	H	1506	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	PO4	P-O2	2.84	1.63	1.53
2	E	1503	PO4	P-O2	3.04	1.64	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1507	PO4	2	0

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	243/290 (83%)	-0.02	10 (4%)	41	40	14, 22, 49, 63	0
1	B	238/290 (82%)	0.10	8 (3%)	49	49	14, 23, 50, 71	0
1	C	243/290 (83%)	0.15	9 (3%)	45	46	13, 26, 52, 82	0
1	D	243/290 (83%)	0.09	10 (4%)	41	40	15, 27, 54, 71	0
1	E	242/290 (83%)	-0.00	5 (2%)	67	70	15, 26, 46, 55	0
1	F	241/290 (83%)	-0.13	5 (2%)	67	70	13, 20, 43, 63	0
1	G	243/290 (83%)	0.07	11 (4%)	37	35	13, 25, 51, 67	0
1	H	243/290 (83%)	-0.12	5 (2%)	67	70	15, 22, 39, 54	0
All	All	1936/2320 (83%)	0.02	63 (3%)	50	51	13, 24, 49, 82	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	247	ASN	6.1
1	C	247	ASN	5.9
1	C	93	ASN	5.4
1	G	229	ALA	4.7
1	A	246	ASP	4.5
1	G	246	ASP	4.5
1	G	231	HIS	4.3
1	G	93	ASN	4.3
1	C	88	GLU	4.0
1	A	57	TYR	3.8
1	D	28	SER	3.7
1	H	171	ASP	3.7
1	G	171	ASP	3.7
1	H	93	ASN	3.6
1	C	246	ASP	3.5
1	H	246	ASP	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	172	ARG	3.5
1	G	230	LYS	3.4
1	A	88	GLU	3.3
1	F	93	ASN	3.3
1	B	52	GLN	3.3
1	E	171	ASP	3.2
1	G	247	ASN	3.2
1	A	245	SER	3.2
1	F	248	ALA	3.1
1	D	88	GLU	3.1
1	H	88	GLU	3.0
1	A	250	GLU	3.0
1	F	247	ASN	2.9
1	B	246	ASP	2.9
1	B	250	GLU	2.8
1	A	52	GLN	2.8
1	D	56	THR	2.8
1	C	56	THR	2.7
1	C	91	ALA	2.7
1	G	169	VAL	2.7
1	F	88	GLU	2.7
1	A	51	GLN	2.7
1	D	55	GLU	2.6
1	C	54	PRO	2.6
1	E	88	GLU	2.6
1	E	93	ASN	2.6
1	G	232	THR	2.4
1	A	89	SER	2.3
1	E	250	GLU	2.3
1	A	91	ALA	2.3
1	D	246	ASP	2.3
1	B	54	PRO	2.3
1	D	51	GLN	2.3
1	F	171	ASP	2.3
1	D	52	GLN	2.2
1	G	276	PRO	2.2
1	D	171	ASP	2.2
1	E	246	ASP	2.2
1	D	54	PRO	2.2
1	D	250	GLU	2.2
1	B	241	ILE	2.1
1	C	245	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	248	ALA	2.1
1	B	88	GLU	2.1
1	C	172	ARG	2.0
1	H	51	GLN	2.0
1	A	231	HIS	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	PO4	C	1507	5/5	0.89	0.15	2.47	19,24,32,33	5
3	MG	A	1508	1/1	0.97	0.08	1.28	32,32,32,32	0
2	PO4	A	1500	5/5	0.98	0.06	-0.45	18,19,21,24	0
2	PO4	D	1502	5/5	0.98	0.06	-0.83	20,21,23,24	0
2	PO4	G	1505	5/5	0.99	0.06	-0.92	17,18,19,22	0
2	PO4	E	1503	5/5	0.98	0.06	-1.00	21,22,24,24	0
2	PO4	B	1501	5/5	0.99	0.06	-1.13	18,18,19,20	0
2	PO4	H	1506	5/5	0.99	0.05	-1.70	17,17,21,21	0
2	PO4	F	1504	5/5	0.99	0.04	-2.43	17,20,20,22	0

6.5 Other polymers (i)

There are no such residues in this entry.