Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:50 AM GMT

PDB ID	:	3N2L
Title	:	2.1 Angstrom resolution crystal structure of an Orotate Phosphoribosyltransferase (pyrE) from Vibrio cholerae O1 biovar eltor str. N16961
Authors	:	Halavaty, A.S.; Minasov, G.; Shuvalova, L.; Dubrovska, I.; Winsor, J.; Kwon, K.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2010-05-18
Resolution	:	2.10 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:

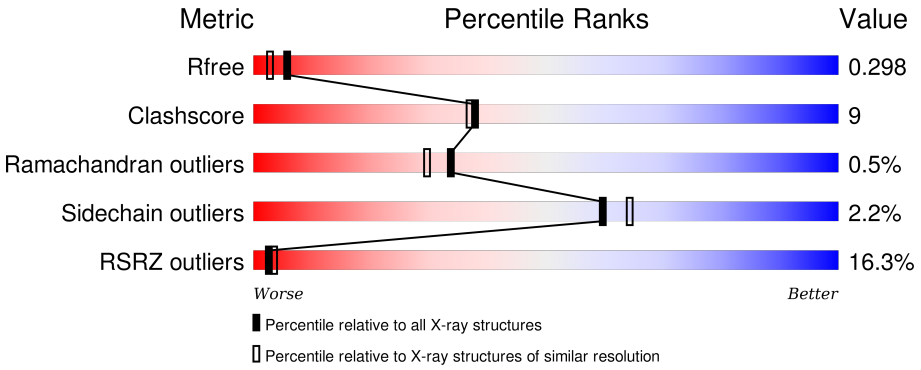
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	238	16% 67% 18% • 14%
1	B	238	13% 58% 14% • 26%
1	C	238	11% 59% 21% • 19%
1	D	238	9% 55% 15% • 29%
1	E	238	15% 65% 19% • 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	238	13% 66% 8% 26%
1	G	238	13% 63% 18% 18%
1	H	238	11% 58% 12% 29%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12436 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 Orotate phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	3	0
			1626	1034	278	309	5			
1	B	175	Total	C	N	O	S	0	1	0
			1377	884	229	258	6			
1	C	193	Total	C	N	O	S	0	3	0
			1546	988	261	291	6			
1	D	170	Total	C	N	O	S	0	0	0
			1330	855	222	248	5			
1	E	205	Total	C	N	O	S	0	3	0
			1626	1037	275	309	5			
1	F	177	Total	C	N	O	S	0	1	0
			1391	893	232	261	5			
1	G	194	Total	C	N	O	S	0	3	0
			1554	991	268	290	5			
1	H	169	Total	C	N	O	S	0	1	0
			1335	860	220	250	5			

There are 200 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	EXPRESSION TAG	UNP Q9KVD5
A	-22	HIS	-	EXPRESSION TAG	UNP Q9KVD5
A	-21	HIS	-	EXPRESSION TAG	UNP Q9KVD5
A	-20	HIS	-	EXPRESSION TAG	UNP Q9KVD5
A	-19	HIS	-	EXPRESSION TAG	UNP Q9KVD5
A	-18	HIS	-	EXPRESSION TAG	UNP Q9KVD5
A	-17	HIS	-	EXPRESSION TAG	UNP Q9KVD5
A	-16	SER	-	EXPRESSION TAG	UNP Q9KVD5
A	-15	SER	-	EXPRESSION TAG	UNP Q9KVD5
A	-14	GLY	-	EXPRESSION TAG	UNP Q9KVD5
A	-13	VAL	-	EXPRESSION TAG	UNP Q9KVD5
A	-12	ASP	-	EXPRESSION TAG	UNP Q9KVD5
A	-11	LEU	-	EXPRESSION TAG	UNP Q9KVD5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	EXPRESSION TAG	UNP Q9KVD5
A	-9	THR	-	EXPRESSION TAG	UNP Q9KVD5
A	-8	GLU	-	EXPRESSION TAG	UNP Q9KVD5
A	-7	ASN	-	EXPRESSION TAG	UNP Q9KVD5
A	-6	LEU	-	EXPRESSION TAG	UNP Q9KVD5
A	-5	TYR	-	EXPRESSION TAG	UNP Q9KVD5
A	-4	PHE	-	EXPRESSION TAG	UNP Q9KVD5
A	-3	GLN	-	EXPRESSION TAG	UNP Q9KVD5
A	-2	SER	-	EXPRESSION TAG	UNP Q9KVD5
A	-1	ASN	-	EXPRESSION TAG	UNP Q9KVD5
A	0	ALA	-	EXPRESSION TAG	UNP Q9KVD5
A	1	MET	-	EXPRESSION TAG	UNP Q9KVD5
B	-23	MET	-	EXPRESSION TAG	UNP Q9KVD5
B	-22	HIS	-	EXPRESSION TAG	UNP Q9KVD5
B	-21	HIS	-	EXPRESSION TAG	UNP Q9KVD5
B	-20	HIS	-	EXPRESSION TAG	UNP Q9KVD5
B	-19	HIS	-	EXPRESSION TAG	UNP Q9KVD5
B	-18	HIS	-	EXPRESSION TAG	UNP Q9KVD5
B	-17	HIS	-	EXPRESSION TAG	UNP Q9KVD5
B	-16	SER	-	EXPRESSION TAG	UNP Q9KVD5
B	-15	SER	-	EXPRESSION TAG	UNP Q9KVD5
B	-14	GLY	-	EXPRESSION TAG	UNP Q9KVD5
B	-13	VAL	-	EXPRESSION TAG	UNP Q9KVD5
B	-12	ASP	-	EXPRESSION TAG	UNP Q9KVD5
B	-11	LEU	-	EXPRESSION TAG	UNP Q9KVD5
B	-10	GLY	-	EXPRESSION TAG	UNP Q9KVD5
B	-9	THR	-	EXPRESSION TAG	UNP Q9KVD5
B	-8	GLU	-	EXPRESSION TAG	UNP Q9KVD5
B	-7	ASN	-	EXPRESSION TAG	UNP Q9KVD5
B	-6	LEU	-	EXPRESSION TAG	UNP Q9KVD5
B	-5	TYR	-	EXPRESSION TAG	UNP Q9KVD5
B	-4	PHE	-	EXPRESSION TAG	UNP Q9KVD5
B	-3	GLN	-	EXPRESSION TAG	UNP Q9KVD5
B	-2	SER	-	EXPRESSION TAG	UNP Q9KVD5
B	-1	ASN	-	EXPRESSION TAG	UNP Q9KVD5
B	0	ALA	-	EXPRESSION TAG	UNP Q9KVD5
B	1	MET	-	EXPRESSION TAG	UNP Q9KVD5
C	-23	MET	-	EXPRESSION TAG	UNP Q9KVD5
C	-22	HIS	-	EXPRESSION TAG	UNP Q9KVD5
C	-21	HIS	-	EXPRESSION TAG	UNP Q9KVD5
C	-20	HIS	-	EXPRESSION TAG	UNP Q9KVD5
C	-19	HIS	-	EXPRESSION TAG	UNP Q9KVD5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	HIS	-	EXPRESSION TAG	UNP Q9KVD5
C	-17	HIS	-	EXPRESSION TAG	UNP Q9KVD5
C	-16	SER	-	EXPRESSION TAG	UNP Q9KVD5
C	-15	SER	-	EXPRESSION TAG	UNP Q9KVD5
C	-14	GLY	-	EXPRESSION TAG	UNP Q9KVD5
C	-13	VAL	-	EXPRESSION TAG	UNP Q9KVD5
C	-12	ASP	-	EXPRESSION TAG	UNP Q9KVD5
C	-11	LEU	-	EXPRESSION TAG	UNP Q9KVD5
C	-10	GLY	-	EXPRESSION TAG	UNP Q9KVD5
C	-9	THR	-	EXPRESSION TAG	UNP Q9KVD5
C	-8	GLU	-	EXPRESSION TAG	UNP Q9KVD5
C	-7	ASN	-	EXPRESSION TAG	UNP Q9KVD5
C	-6	LEU	-	EXPRESSION TAG	UNP Q9KVD5
C	-5	TYR	-	EXPRESSION TAG	UNP Q9KVD5
C	-4	PHE	-	EXPRESSION TAG	UNP Q9KVD5
C	-3	GLN	-	EXPRESSION TAG	UNP Q9KVD5
C	-2	SER	-	EXPRESSION TAG	UNP Q9KVD5
C	-1	ASN	-	EXPRESSION TAG	UNP Q9KVD5
C	0	ALA	-	EXPRESSION TAG	UNP Q9KVD5
C	1	MET	-	EXPRESSION TAG	UNP Q9KVD5
D	-23	MET	-	EXPRESSION TAG	UNP Q9KVD5
D	-22	HIS	-	EXPRESSION TAG	UNP Q9KVD5
D	-21	HIS	-	EXPRESSION TAG	UNP Q9KVD5
D	-20	HIS	-	EXPRESSION TAG	UNP Q9KVD5
D	-19	HIS	-	EXPRESSION TAG	UNP Q9KVD5
D	-18	HIS	-	EXPRESSION TAG	UNP Q9KVD5
D	-17	HIS	-	EXPRESSION TAG	UNP Q9KVD5
D	-16	SER	-	EXPRESSION TAG	UNP Q9KVD5
D	-15	SER	-	EXPRESSION TAG	UNP Q9KVD5
D	-14	GLY	-	EXPRESSION TAG	UNP Q9KVD5
D	-13	VAL	-	EXPRESSION TAG	UNP Q9KVD5
D	-12	ASP	-	EXPRESSION TAG	UNP Q9KVD5
D	-11	LEU	-	EXPRESSION TAG	UNP Q9KVD5
D	-10	GLY	-	EXPRESSION TAG	UNP Q9KVD5
D	-9	THR	-	EXPRESSION TAG	UNP Q9KVD5
D	-8	GLU	-	EXPRESSION TAG	UNP Q9KVD5
D	-7	ASN	-	EXPRESSION TAG	UNP Q9KVD5
D	-6	LEU	-	EXPRESSION TAG	UNP Q9KVD5
D	-5	TYR	-	EXPRESSION TAG	UNP Q9KVD5
D	-4	PHE	-	EXPRESSION TAG	UNP Q9KVD5
D	-3	GLN	-	EXPRESSION TAG	UNP Q9KVD5
D	-2	SER	-	EXPRESSION TAG	UNP Q9KVD5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	ASN	-	EXPRESSION TAG	UNP Q9KVD5
D	0	ALA	-	EXPRESSION TAG	UNP Q9KVD5
D	1	MET	-	EXPRESSION TAG	UNP Q9KVD5
E	-23	MET	-	EXPRESSION TAG	UNP Q9KVD5
E	-22	HIS	-	EXPRESSION TAG	UNP Q9KVD5
E	-21	HIS	-	EXPRESSION TAG	UNP Q9KVD5
E	-20	HIS	-	EXPRESSION TAG	UNP Q9KVD5
E	-19	HIS	-	EXPRESSION TAG	UNP Q9KVD5
E	-18	HIS	-	EXPRESSION TAG	UNP Q9KVD5
E	-17	HIS	-	EXPRESSION TAG	UNP Q9KVD5
E	-16	SER	-	EXPRESSION TAG	UNP Q9KVD5
E	-15	SER	-	EXPRESSION TAG	UNP Q9KVD5
E	-14	GLY	-	EXPRESSION TAG	UNP Q9KVD5
E	-13	VAL	-	EXPRESSION TAG	UNP Q9KVD5
E	-12	ASP	-	EXPRESSION TAG	UNP Q9KVD5
E	-11	LEU	-	EXPRESSION TAG	UNP Q9KVD5
E	-10	GLY	-	EXPRESSION TAG	UNP Q9KVD5
E	-9	THR	-	EXPRESSION TAG	UNP Q9KVD5
E	-8	GLU	-	EXPRESSION TAG	UNP Q9KVD5
E	-7	ASN	-	EXPRESSION TAG	UNP Q9KVD5
E	-6	LEU	-	EXPRESSION TAG	UNP Q9KVD5
E	-5	TYR	-	EXPRESSION TAG	UNP Q9KVD5
E	-4	PHE	-	EXPRESSION TAG	UNP Q9KVD5
E	-3	GLN	-	EXPRESSION TAG	UNP Q9KVD5
E	-2	SER	-	EXPRESSION TAG	UNP Q9KVD5
E	-1	ASN	-	EXPRESSION TAG	UNP Q9KVD5
E	0	ALA	-	EXPRESSION TAG	UNP Q9KVD5
E	1	MET	-	EXPRESSION TAG	UNP Q9KVD5
F	-23	MET	-	EXPRESSION TAG	UNP Q9KVD5
F	-22	HIS	-	EXPRESSION TAG	UNP Q9KVD5
F	-21	HIS	-	EXPRESSION TAG	UNP Q9KVD5
F	-20	HIS	-	EXPRESSION TAG	UNP Q9KVD5
F	-19	HIS	-	EXPRESSION TAG	UNP Q9KVD5
F	-18	HIS	-	EXPRESSION TAG	UNP Q9KVD5
F	-17	HIS	-	EXPRESSION TAG	UNP Q9KVD5
F	-16	SER	-	EXPRESSION TAG	UNP Q9KVD5
F	-15	SER	-	EXPRESSION TAG	UNP Q9KVD5
F	-14	GLY	-	EXPRESSION TAG	UNP Q9KVD5
F	-13	VAL	-	EXPRESSION TAG	UNP Q9KVD5
F	-12	ASP	-	EXPRESSION TAG	UNP Q9KVD5
F	-11	LEU	-	EXPRESSION TAG	UNP Q9KVD5
F	-10	GLY	-	EXPRESSION TAG	UNP Q9KVD5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-9	THR	-	EXPRESSION TAG	UNP Q9KVD5
F	-8	GLU	-	EXPRESSION TAG	UNP Q9KVD5
F	-7	ASN	-	EXPRESSION TAG	UNP Q9KVD5
F	-6	LEU	-	EXPRESSION TAG	UNP Q9KVD5
F	-5	TYR	-	EXPRESSION TAG	UNP Q9KVD5
F	-4	PHE	-	EXPRESSION TAG	UNP Q9KVD5
F	-3	GLN	-	EXPRESSION TAG	UNP Q9KVD5
F	-2	SER	-	EXPRESSION TAG	UNP Q9KVD5
F	-1	ASN	-	EXPRESSION TAG	UNP Q9KVD5
F	0	ALA	-	EXPRESSION TAG	UNP Q9KVD5
F	1	MET	-	EXPRESSION TAG	UNP Q9KVD5
G	-23	MET	-	EXPRESSION TAG	UNP Q9KVD5
G	-22	HIS	-	EXPRESSION TAG	UNP Q9KVD5
G	-21	HIS	-	EXPRESSION TAG	UNP Q9KVD5
G	-20	HIS	-	EXPRESSION TAG	UNP Q9KVD5
G	-19	HIS	-	EXPRESSION TAG	UNP Q9KVD5
G	-18	HIS	-	EXPRESSION TAG	UNP Q9KVD5
G	-17	HIS	-	EXPRESSION TAG	UNP Q9KVD5
G	-16	SER	-	EXPRESSION TAG	UNP Q9KVD5
G	-15	SER	-	EXPRESSION TAG	UNP Q9KVD5
G	-14	GLY	-	EXPRESSION TAG	UNP Q9KVD5
G	-13	VAL	-	EXPRESSION TAG	UNP Q9KVD5
G	-12	ASP	-	EXPRESSION TAG	UNP Q9KVD5
G	-11	LEU	-	EXPRESSION TAG	UNP Q9KVD5
G	-10	GLY	-	EXPRESSION TAG	UNP Q9KVD5
G	-9	THR	-	EXPRESSION TAG	UNP Q9KVD5
G	-8	GLU	-	EXPRESSION TAG	UNP Q9KVD5
G	-7	ASN	-	EXPRESSION TAG	UNP Q9KVD5
G	-6	LEU	-	EXPRESSION TAG	UNP Q9KVD5
G	-5	TYR	-	EXPRESSION TAG	UNP Q9KVD5
G	-4	PHE	-	EXPRESSION TAG	UNP Q9KVD5
G	-3	GLN	-	EXPRESSION TAG	UNP Q9KVD5
G	-2	SER	-	EXPRESSION TAG	UNP Q9KVD5
G	-1	ASN	-	EXPRESSION TAG	UNP Q9KVD5
G	0	ALA	-	EXPRESSION TAG	UNP Q9KVD5
G	1	MET	-	EXPRESSION TAG	UNP Q9KVD5
H	-23	MET	-	EXPRESSION TAG	UNP Q9KVD5
H	-22	HIS	-	EXPRESSION TAG	UNP Q9KVD5
H	-21	HIS	-	EXPRESSION TAG	UNP Q9KVD5
H	-20	HIS	-	EXPRESSION TAG	UNP Q9KVD5
H	-19	HIS	-	EXPRESSION TAG	UNP Q9KVD5
H	-18	HIS	-	EXPRESSION TAG	UNP Q9KVD5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	-17	HIS	-	EXPRESSION TAG	UNP Q9KVD5
H	-16	SER	-	EXPRESSION TAG	UNP Q9KVD5
H	-15	SER	-	EXPRESSION TAG	UNP Q9KVD5
H	-14	GLY	-	EXPRESSION TAG	UNP Q9KVD5
H	-13	VAL	-	EXPRESSION TAG	UNP Q9KVD5
H	-12	ASP	-	EXPRESSION TAG	UNP Q9KVD5
H	-11	LEU	-	EXPRESSION TAG	UNP Q9KVD5
H	-10	GLY	-	EXPRESSION TAG	UNP Q9KVD5
H	-9	THR	-	EXPRESSION TAG	UNP Q9KVD5
H	-8	GLU	-	EXPRESSION TAG	UNP Q9KVD5
H	-7	ASN	-	EXPRESSION TAG	UNP Q9KVD5
H	-6	LEU	-	EXPRESSION TAG	UNP Q9KVD5
H	-5	TYR	-	EXPRESSION TAG	UNP Q9KVD5
H	-4	PHE	-	EXPRESSION TAG	UNP Q9KVD5
H	-3	GLN	-	EXPRESSION TAG	UNP Q9KVD5
H	-2	SER	-	EXPRESSION TAG	UNP Q9KVD5
H	-1	ASN	-	EXPRESSION TAG	UNP Q9KVD5
H	0	ALA	-	EXPRESSION TAG	UNP Q9KVD5
H	1	MET	-	EXPRESSION TAG	UNP Q9KVD5

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	2	Total Cl 2 2	0	0
2	A	1	Total Cl 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	95	Total O 96 96	0	1
3	B	82	Total O 83 83	0	2
3	C	78	Total O 79 79	0	1
3	D	71	Total O 74 74	0	3
3	E	100	Total O 101 101	0	3
3	F	68	Total O 69 69	0	1

Continued on next page...

Continued from previous page...

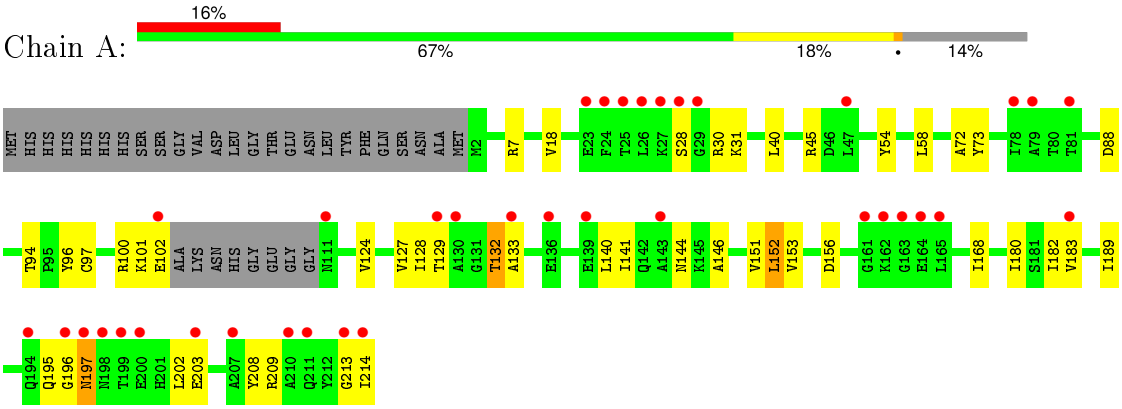
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	74	Total O 74 74	0	1
3	H	71	Total O 72 72	0	1

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.

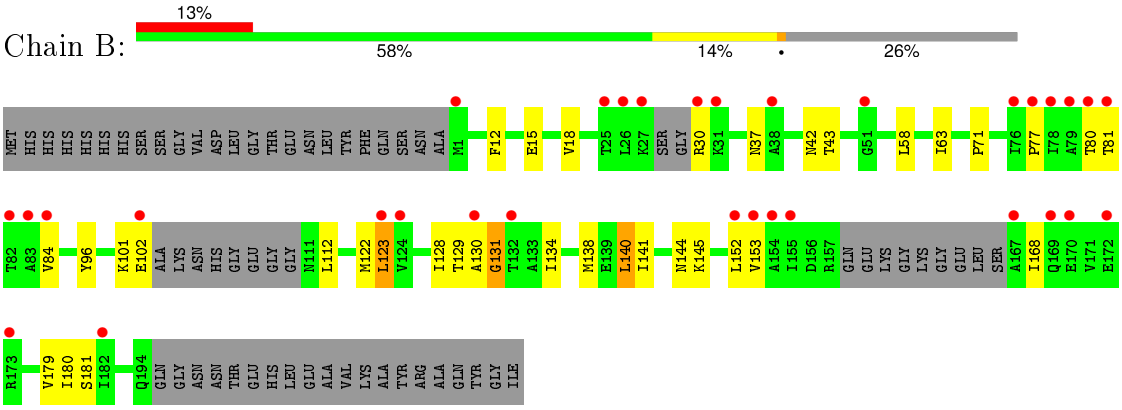
- Molecule 1: Orotate phosphoribosyltransferase

Chain A:



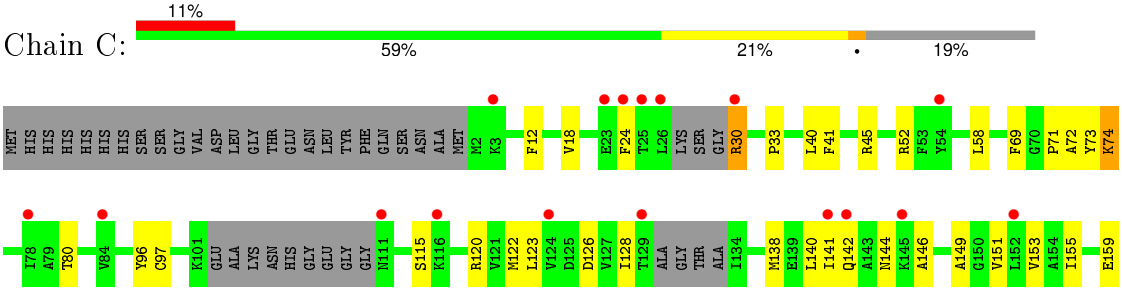
- Molecule 1: Orotate phosphoribosyltransferase

Chain B:

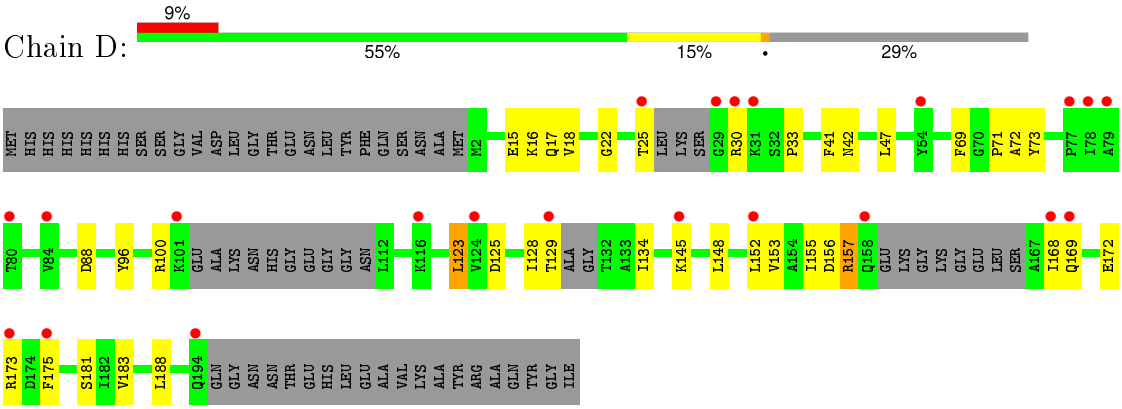


- Molecule 1: Orotate phosphoribosyltransferase

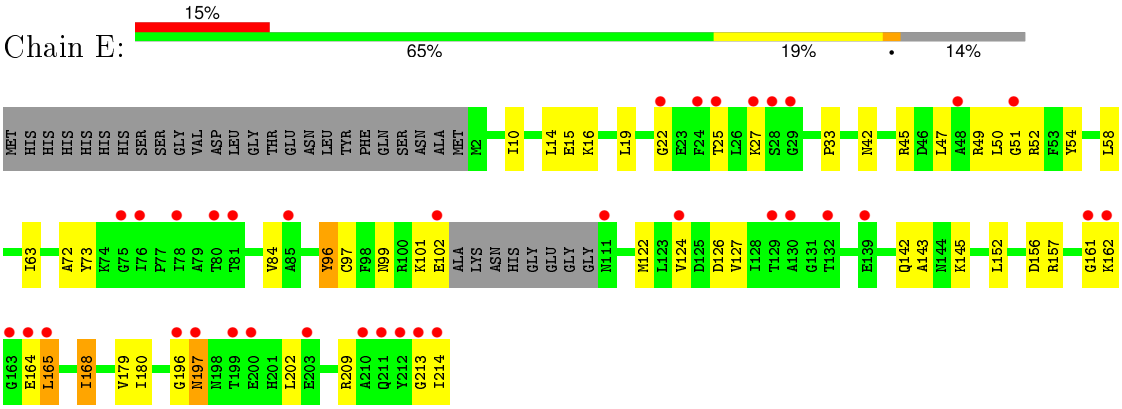
Chain C:



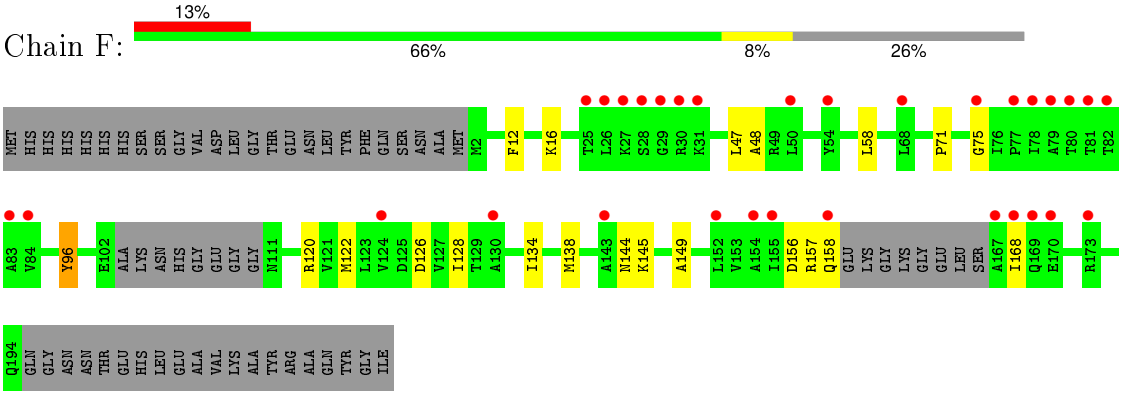
• Molecule 1: Orotate phosphoribosyltransferase



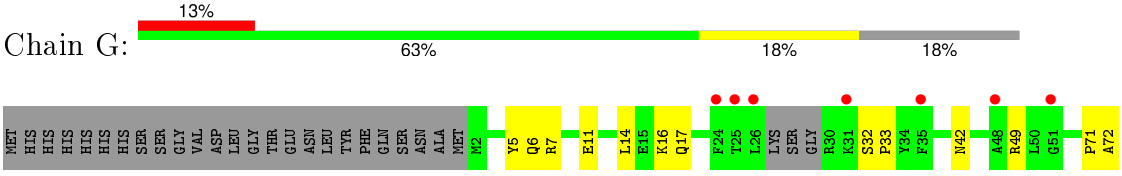
• Molecule 1: Orotate phosphoribosyltransferase

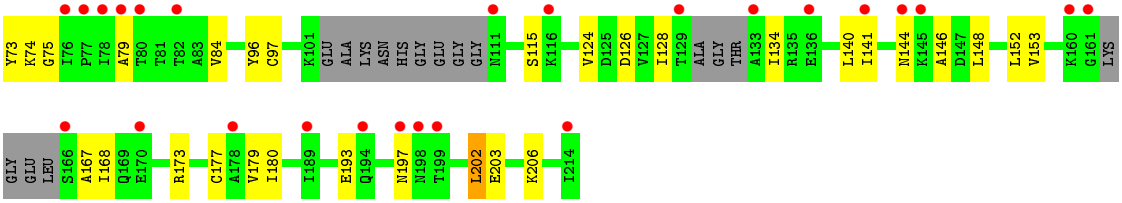


• Molecule 1: Orotate phosphoribosyltransferase



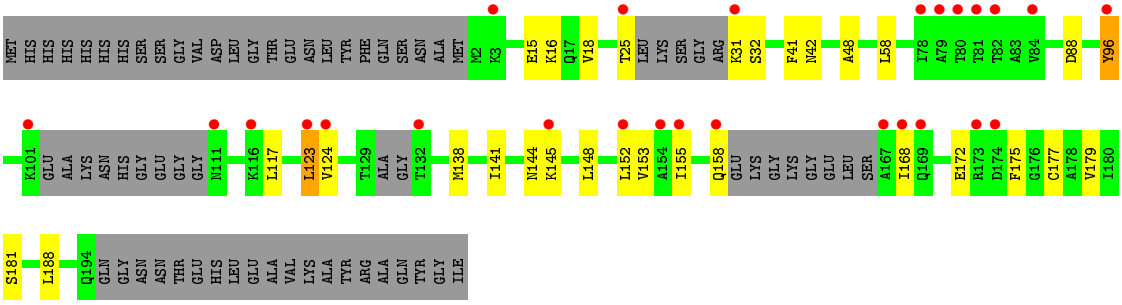
• Molecule 1: Orotate phosphoribosyltransferase





- Molecule 1: Orotate phosphoribosyltransferase

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	96.59Å 76.71Å 133.94Å 90.00° 92.63° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 29.66 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-2.10) 99.5 (29.66-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.222 , 0.269 0.259 , 0.298	Depositor DCC
R_{free} test set	5709 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	32.2	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.5	EDS
Estimated twinning fraction	0.052 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 114007 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12436	wwPDB-VP
Average B, all atoms (Å^2)	44.0	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 89.09 % 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 3.8806e-08.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

Bond lengths and bond angles in the following residue types are not validated in this section: CL

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	0.79	1/1651 (0.1%)	0.90	2/2222 (0.1%)
1	B	0.72	0/1397	0.81	1/1882 (0.1%)
1	C	0.67	0/1568	0.78	2/2109 (0.1%)
1	D	0.71	1/1349 (0.1%)	0.84	2/1817 (0.1%)
1	E	0.77	2/1652 (0.1%)	0.85	4/2224 (0.2%)
1	F	0.71	0/1413	0.81	2/1906 (0.1%)
1	G	0.69	1/1576 (0.1%)	0.77	2/2118 (0.1%)
1	H	0.68	0/1355	0.79	3/1827 (0.2%)
All	All	0.72	5/11961 (0.0%)	0.82	18/16105 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	97	CYS	CB-SG	-7.74	1.69	1.82
1	A	97	CYS	CB-SG	-7.16	1.70	1.82
1	D	15	GLU	CG-CD	6.38	1.61	1.51
1	G	97	CYS	CB-SG	-5.15	1.73	1.81
1	E	51	GLY	N-CA	-5.02	1.38	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	164	GLU	CB-CA-C	-9.68	91.04	110.40
1	A	88	ASP	CB-CG-OD2	-9.63	109.63	118.30
1	A	88	ASP	CB-CG-OD1	8.40	125.86	118.30
1	F	126	ASP	CB-CG-OD1	6.70	124.33	118.30
1	E	164	GLU	N-CA-C	6.33	128.10	111.00
1	D	88	ASP	CB-CG-OD1	6.09	123.78	118.30
1	G	49	ARG	NE-CZ-NH1	-6.09	117.26	120.30
1	E	165	LEU	N-CA-CB	6.07	122.55	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	156	ASP	CB-CA-C	-5.80	98.80	110.40
1	H	123	LEU	CA-CB-CG	5.76	128.55	115.30
1	E	52	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	123	LEU	CA-CB-CG	5.51	127.97	115.30
1	G	49	ARG	NE-CZ-NH2	5.45	123.03	120.30
1	C	24	PHE	CB-CA-C	-5.31	99.78	110.40
1	C	52	ARG	NE-CZ-NH2	5.19	122.89	120.30
1	H	88	ASP	CB-CG-OD1	5.10	122.89	118.30
1	D	123	LEU	CA-CB-CG	5.06	126.94	115.30
1	H	58	LEU	CB-CG-CD2	-5.00	102.50	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1626	0	1623	40	0
1	B	1377	0	1383	25	0
1	C	1546	0	1540	41	0
1	D	1330	0	1332	23	0
1	E	1626	0	1619	36	0
1	F	1391	0	1391	15	0
1	G	1554	0	1552	32	0
1	H	1335	0	1330	24	0
2	A	1	0	0	1	0
2	H	2	0	0	0	0
3	A	96	0	0	4	0
3	B	83	0	0	0	0
3	C	79	0	0	1	0
3	D	74	0	0	0	0
3	E	101	0	0	1	0
3	F	69	0	0	0	0
3	G	74	0	0	1	0
3	H	72	0	0	1	0
All	All	12436	0	11770	218	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 9.

All (218) 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:69:PHE:HD1	1:C:97[B]:CYS:HG	0.96	0.90
1:C:69:PHE:HD1	1:C:97[B]:CYS:SG	1.99	0.85
1:E:15:GLU:OE1	1:E:16:LYS:HE2	1.80	0.81
1:G:140:LEU:O	1:G:144:ASN:ND2	2.21	0.73
1:E:84:VAL:HG13	1:F:48:ALA:HB2	1.76	0.67
1:B:101:LYS:O	1:B:102:GLU:C	2.32	0.66
1:H:145:LYS:HG2	1:H:145:LYS:O	1.96	0.66
1:A:18:VAL:HG22	1:A:40:LEU:HB2	1.80	0.64
1:A:214:ILE:HD12	1:A:214:ILE:N	2.12	0.63
1:E:15:GLU:OE1	1:E:49:ARG:NH2	2.32	0.63
1:E:58:LEU:HG	1:E:152:LEU:HD22	1.80	0.63
1:A:152:LEU:HD23	1:A:153:VAL:O	1.99	0.63
1:D:168:ILE:HG13	1:D:169:GLN:N	2.12	0.63
1:D:30:ARG:HD3	1:D:129:THR:HG21	1.81	0.62
1:E:10:ILE:O	1:E:14:LEU:HG	1.98	0.62
1:D:25:THR:C	1:D:30:ARG:O	2.38	0.62
1:A:152:LEU:HD23	1:A:153:VAL:N	2.15	0.61
1:E:84:VAL:HG13	1:F:48:ALA:CB	2.30	0.61
1:F:157:ARG:O	1:F:158:GLN:HB2	2.01	0.60
1:C:195:GLN:O	1:C:196:GLY:O	2.19	0.60
1:G:202:LEU:HD21	1:G:206:LYS:HE3	1.83	0.60
1:A:196:GLY:O	1:A:197:ASN:C	2.40	0.60
1:D:148:LEU:HD13	1:D:175:PHE:HB3	1.84	0.59
1:A:182:ILE:HG22	1:A:183:VAL:HG13	1.84	0.59
1:E:45:ARG:NH1	3:E:596:HOH:O	2.28	0.59
1:G:128:ILE:HG22	1:G:167:ALA:HB1	1.84	0.59
1:G:202:LEU:C	1:G:202:LEU:HD23	2.23	0.59
1:B:112:LEU:HD21	1:B:140:LEU:HD21	1.85	0.58
1:B:63:ILE:HD12	1:B:180:ILE:HD13	1.84	0.58
1:C:189:ILE:HD12	1:C:190:THR:N	2.18	0.58
1:B:168:ILE:HG23	1:B:179:VAL:HB	1.85	0.58
1:A:124:VAL:HG12	1:A:152:LEU:HB3	1.85	0.58
1:D:71:PRO:HG3	1:D:123:LEU:HD22	1.86	0.58
1:E:209:ARG:O	1:E:213:GLY:N	2.37	0.58
1:B:128:ILE:HD12	1:B:134:ILE:HD13	1.86	0.57
1:A:152:LEU:HA	1:A:180:ILE:O	2.03	0.57
1:H:155:ILE:CD1	1:H:188:LEU:HD11	2.33	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:ARG:NH2	1:C:174:ASP:OD1	2.37	0.57
1:C:128:ILE:HD12	1:C:168:ILE:HG12	1.86	0.57
1:C:189:ILE:HD12	1:C:189:ILE:C	2.24	0.57
1:G:16:LYS:O	1:G:17:GLN:HB2	2.04	0.57
1:H:158:GLN:NE2	3:H:239:HOH:O	2.37	0.57
1:C:202:LEU:HD23	1:C:202:LEU:C	2.26	0.56
1:C:140:LEU:O	1:C:144:ASN:ND2	2.25	0.56
1:E:101:LYS:O	1:E:102:GLU:C	2.44	0.56
1:E:168:ILE:HG12	1:E:179:VAL:HG11	1.87	0.55
1:D:128:ILE:HG12	1:D:134:ILE:HD12	1.88	0.55
1:H:144:ASN:O	1:H:145:LYS:HB3	2.06	0.55
1:C:30:ARG:NH2	1:C:159:GLU:OE1	2.39	0.55
1:G:202:LEU:O	1:G:202:LEU:HD23	2.06	0.55
1:C:74[A]:LYS:HZ2	1:C:126:ASP:HB3	1.70	0.55
1:B:123:LEU:HD11	1:B:141:ILE:HD12	1.88	0.55
1:G:16:LYS:HE3	3:G:227:HOH:O	2.07	0.54
1:A:202:LEU:HD23	1:A:203:GLU:OE1	2.08	0.54
1:G:42:ASN:HA	1:H:96[B]:TYR:CE2	2.43	0.53
1:C:128:ILE:HD12	1:C:179:VAL:HG11	1.90	0.53
1:A:58:LEU:HG	1:A:152:LEU:HD12	1.91	0.53
1:E:202:LEU:O	1:E:202:LEU:HD23	2.09	0.53
1:E:162:LYS:HA	1:E:162:LYS:HE2	1.91	0.53
1:C:209:ARG:O	1:C:213:GLY:N	2.40	0.52
1:G:84:VAL:HG13	1:H:48:ALA:HB2	1.91	0.52
1:E:14:LEU:CD2	1:E:19:LEU:HD23	2.39	0.52
1:A:140:LEU:O	1:A:144:ASN:ND2	2.32	0.52
1:G:202:LEU:CD2	1:G:202:LEU:C	2.78	0.52
1:D:153:VAL:O	1:D:181:SER:HA	2.09	0.52
1:D:69:PHE:CD2	1:D:123:LEU:HD23	2.45	0.52
1:B:153:VAL:O	1:B:181:SER:HA	2.09	0.52
1:D:168:ILE:HG13	1:D:169:GLN:H	1.73	0.51
1:E:25:THR:HG23	1:E:25:THR:O	2.10	0.51
1:E:124:VAL:HG12	1:E:152:LEU:HB3	1.92	0.51
1:G:128:ILE:HD12	1:G:179:VAL:HG11	1.92	0.51
1:C:71:PRO:CG	1:C:123:LEU:HD21	2.41	0.51
1:B:134:ILE:HG22	1:B:138:MET:SD	2.51	0.51
1:A:7:ARG:NH2	3:A:498:HOH:O	2.38	0.51
1:C:186:THR:O	1:C:189:ILE:HG13	2.10	0.50
1:H:25:THR:HA	1:H:31:LYS:HA	1.93	0.50
1:E:156:ASP:CG	1:E:168:ILE:HD12	2.32	0.50
1:C:138:MET:HG3	1:C:175:PHE:CE1	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:LEU:HD11	1:G:193:GLU:HG2	1.94	0.50
1:C:45:ARG:NH2	3:C:595:HOH:O	2.44	0.50
1:C:151:VAL:HG23	1:C:177:CYS:SG	2.51	0.50
1:E:22:GLY:O	1:E:33:PRO:HA	2.11	0.50
1:E:161:GLY:O	1:E:162:LYS:C	2.48	0.49
1:E:63:ILE:HD12	1:E:180:ILE:HD11	1.94	0.49
1:G:74[A]:LYS:HG2	1:G:126:ASP:CG	2.33	0.49
1:H:123:LEU:HD11	1:H:138:MET:HG3	1.94	0.49
1:B:123:LEU:HD11	1:B:141:ILE:CD1	2.42	0.49
1:B:71:PRO:HG3	1:B:123:LEU:HD23	1.94	0.49
1:C:128:ILE:HG13	1:C:153:VAL:HG11	1.94	0.49
1:E:42:ASN:HA	1:F:96[B]:TYR:CE2	2.48	0.49
1:E:14:LEU:HD21	1:E:19:LEU:HD23	1.94	0.49
1:A:45[B]:ARG:NH1	3:A:246:HOH:O	2.46	0.49
1:B:128:ILE:C	1:B:130:ALA:H	2.16	0.48
1:G:11:GLU:HA	1:G:14:LEU:HD12	1.93	0.48
1:A:101:LYS:O	1:A:102:GLU:HG3	2.13	0.48
1:F:128:ILE:HG13	1:F:128:ILE:O	2.14	0.48
1:H:148:LEU:HD13	1:H:175:PHE:HB3	1.96	0.48
1:C:128:ILE:CD1	1:C:179:VAL:HG11	2.43	0.48
1:A:30:ARG:HD3	1:C:212:TYR:CE1	2.49	0.48
1:A:152:LEU:CD2	1:A:153:VAL:O	2.61	0.48
1:C:138:MET:HG3	1:C:175:PHE:CZ	2.49	0.47
1:B:128:ILE:HD12	1:B:134:ILE:CD1	2.44	0.47
1:E:214:ILE:HD12	1:E:214:ILE:N	2.29	0.47
1:A:127:VAL:HG23	1:A:129:THR:HG23	1.96	0.47
1:C:155:ILE:HA	1:C:183:VAL:O	2.15	0.47
1:A:101:LYS:O	1:A:102:GLU:CG	2.63	0.47
1:E:96:TYR:CZ	1:F:47:LEU:HD11	2.49	0.47
1:C:165:LEU:O	1:C:165:LEU:HD12	2.15	0.47
1:E:27:LYS:HD2	1:E:27:LYS:H	1.80	0.47
1:B:30:ARG:HB3	1:B:30:ARG:NH1	2.30	0.47
1:B:80:THR:O	1:B:84:VAL:HG23	2.15	0.47
1:H:155:ILE:HD11	1:H:188:LEU:HD11	1.97	0.47
1:B:129:THR:C	1:B:131:GLY:H	2.19	0.46
1:A:54:TYR:CD2	1:A:152:LEU:HD22	2.49	0.46
1:H:153:VAL:O	1:H:181:SER:HA	2.15	0.46
1:A:45[B]:ARG:NE	3:A:218:HOH:O	2.36	0.46
1:A:168:ILE:HG13	3:A:261:HOH:O	2.16	0.46
1:A:152:LEU:HG	1:A:180:ILE:HG22	1.97	0.46
1:G:84:VAL:HG13	1:H:48:ALA:CB	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:LYS:HE3	1:D:145:LYS:HB2	1.69	0.46
1:C:58:LEU:HD21	1:C:122:MET:HG2	1.98	0.46
1:C:141:ILE:HG23	1:C:146:ALA:HB3	1.98	0.46
1:A:54:TYR:CE2	1:A:152:LEU:HD22	2.52	0.45
1:G:148:LEU:HD21	1:G:177:CYS:SG	2.57	0.45
1:E:202:LEU:HD11	1:G:193:GLU:CG	2.46	0.45
1:B:58:LEU:HD11	1:B:122:MET:HG2	1.98	0.45
1:A:128:ILE:HG13	1:A:153:VAL:HG11	1.98	0.45
1:F:157:ARG:O	1:F:158:GLN:CB	2.64	0.45
1:B:128:ILE:C	1:B:130:ALA:N	2.69	0.45
1:G:42:ASN:C	1:H:96[B]:TYR:CE2	2.90	0.45
1:A:72:ALA:HA	1:A:73:TYR:HA	1.82	0.45
1:A:132:THR:HG23	1:A:133:ALA:H	1.82	0.45
1:B:12:PHE:O	1:B:15[B]:GLU:HG2	2.15	0.45
1:H:18:VAL:HG21	1:H:41:PHE:CE1	2.51	0.45
1:A:209:ARG:O	1:A:213:GLY:N	2.47	0.45
1:B:152:LEU:HD13	1:B:180:ILE:HG13	1.99	0.45
1:C:202:LEU:HD23	1:C:202:LEU:O	2.16	0.45
1:H:123:LEU:HD21	1:H:141:ILE:CD1	2.47	0.45
1:D:18:VAL:HG21	1:D:41:PHE:CD1	2.52	0.45
1:F:128:ILE:HG21	1:F:168:ILE:HG12	1.98	0.44
1:E:145:LYS:HD3	1:E:145:LYS:N	2.32	0.44
1:G:128:ILE:HB	1:G:168:ILE:HD12	2.00	0.44
1:H:155:ILE:HD12	1:H:188:LEU:HD11	1.99	0.44
1:H:15:GLU:HG3	1:H:16:LYS:HE3	1.99	0.44
1:H:117:LEU:HA	1:H:117:LEU:HD12	1.83	0.44
1:H:172:GLU:HG2	1:H:177:CYS:O	2.18	0.44
1:A:182:ILE:C	1:A:183:VAL:HG13	2.37	0.44
1:C:18:VAL:HG22	1:C:40:LEU:HB2	1.99	0.44
1:C:69:PHE:CD1	1:C:97[B]:CYS:SG	2.90	0.44
1:C:202:LEU:CD2	1:C:202:LEU:C	2.86	0.44
1:H:168:ILE:CG2	1:H:179:VAL:HG11	2.47	0.44
1:G:16:LYS:O	1:G:17:GLN:CB	2.66	0.43
1:A:180:ILE:HA	1:A:180:ILE:HD13	1.79	0.43
1:H:18:VAL:HG21	1:H:41:PHE:CD1	2.52	0.43
1:G:72:ALA:HA	1:G:73:TYR:HA	1.82	0.43
1:F:128:ILE:HD12	1:F:134:ILE:HD13	2.01	0.43
1:F:12:PHE:O	1:F:16:LYS:HG3	2.19	0.43
1:E:58:LEU:HD21	1:E:122:MET:HG2	2.00	0.43
1:C:165:LEU:HD12	1:C:165:LEU:C	2.39	0.43
1:F:144:ASN:O	1:F:145:LYS:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:ALA:HA	1:E:73:TYR:HA	1.75	0.43
1:G:71:PRO:HD2	1:G:75:GLY:HA3	2.00	0.43
1:B:77:PRO:O	1:B:81:THR:HG22	2.18	0.43
1:D:156:ASP:HB2	1:D:157:ARG:NH2	2.33	0.43
1:A:213:GLY:C	1:A:214:ILE:HD12	2.39	0.43
1:A:94:THR:O	1:A:94:THR:HG23	2.18	0.43
1:A:141:ILE:HG23	1:A:146:ALA:HB3	2.00	0.43
1:G:152:LEU:HD13	1:G:180:ILE:HG13	2.01	0.43
1:D:152:LEU:HD12	1:D:181:SER:HA	1.99	0.43
1:G:128:ILE:CD1	1:G:179:VAL:HG11	2.49	0.42
1:A:156:ASP:CG	1:A:168:ILE:HD12	2.40	0.42
1:B:18:VAL:HG13	1:B:37:ASN:O	2.19	0.42
1:G:5:TYR:CE1	1:G:6:GLN:HG3	2.54	0.42
1:E:47:LEU:HD11	1:F:96[B]:TYR:CE2	2.54	0.42
1:F:58:LEU:HD11	1:F:122:MET:HG2	2.01	0.42
1:A:128:ILE:HD11	1:A:151:VAL:HG11	2.00	0.42
1:G:115:SER:HB2	1:H:42:ASN:HB2	2.01	0.42
1:E:165:LEU:HD23	1:E:165:LEU:HA	1.94	0.42
1:G:79:ALA:HA	1:G:124:VAL:HG21	2.01	0.42
1:C:80:THR:HG23	1:D:47:LEU:HD13	2.01	0.42
1:G:32:SER:OG	1:G:33:PRO:HD2	2.18	0.42
1:A:100:ARG:NH1	2:A:215:CL:CL	2.79	0.42
1:C:12:PHE:CE2	1:C:41:PHE:CE1	3.08	0.42
1:A:31:LYS:N	1:A:31:LYS:HD2	2.34	0.42
1:A:141:ILE:HG22	1:A:146:ALA:O	2.19	0.42
1:C:138:MET:HG3	1:C:175:PHE:CD1	2.55	0.42
1:D:16:LYS:O	1:D:17:GLN:HB2	2.20	0.42
1:A:189:ILE:CD1	1:C:209:ARG:HD3	2.50	0.41
1:H:148:LEU:CD1	1:H:175:PHE:HB3	2.49	0.41
1:F:120:ARG:HB3	1:F:149:ALA:HB2	2.02	0.41
1:B:42:ASN:OD1	1:B:43:THR:HG23	2.20	0.41
1:H:124:VAL:HG12	1:H:152:LEU:HB3	2.01	0.41
1:E:50:LEU:HD11	1:E:54:TYR:HE1	1.85	0.41
1:D:72:ALA:HA	1:D:73:TYR:HA	1.83	0.41
1:E:196:GLY:O	1:E:197:ASN:C	2.59	0.41
1:G:202:LEU:HD22	1:G:203:GLU:CD	2.41	0.41
1:D:69:PHE:HD2	1:D:123:LEU:HD23	1.83	0.41
1:B:128:ILE:HG21	1:B:168:ILE:HG13	2.02	0.41
1:C:72:ALA:HA	1:C:73:TYR:HA	1.82	0.41
1:G:128:ILE:HG13	1:G:153:VAL:HG11	2.02	0.41
1:B:144:ASN:O	1:B:145:LYS:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:GLU:OE1	1:A:203:GLU:HA	2.21	0.41
1:D:125:ASP:O	1:D:153:VAL:HA	2.20	0.41
1:A:208:TYR:CD1	1:C:33:PRO:HD3	2.56	0.41
1:G:141:ILE:HG23	1:G:146:ALA:HB3	2.02	0.41
1:E:126:ASP:OD1	1:E:127:VAL:N	2.49	0.41
1:C:120:ARG:HB3	1:C:149:ALA:HB2	2.02	0.41
1:E:72:ALA:HB2	1:E:99:ASN:O	2.20	0.40
1:E:142:GLN:HG3	1:E:143:ALA:N	2.35	0.40
1:G:202:LEU:HD21	1:G:206:LYS:CE	2.50	0.40
1:C:74[B]:LYS:HE3	1:D:100:ARG:HH22	1.86	0.40
1:D:22:GLY:O	1:D:33:PRO:HA	2.22	0.40
1:C:71:PRO:HG3	1:C:123:LEU:HD21	2.02	0.40
1:C:115:SER:HB2	1:D:42:ASN:HB2	2.03	0.40
1:F:71:PRO:HD2	1:F:75:GLY:HA3	2.04	0.40
1:B:168:ILE:HG23	1:B:179:VAL:CB	2.49	0.40
1:D:155:ILE:HD12	1:D:188:LEU:HD11	2.03	0.40
1:D:155:ILE:HA	1:D:183:VAL:O	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	204/238 (86%)	197 (97%)	5 (2%)	2 (1%)	19 13
1	B	168/238 (71%)	164 (98%)	3 (2%)	1 (1%)	30 24
1	C	186/238 (78%)	182 (98%)	2 (1%)	2 (1%)	17 11
1	D	160/238 (67%)	157 (98%)	3 (2%)	0	100 100
1	E	204/238 (86%)	196 (96%)	7 (3%)	1 (0%)	34 30
1	F	172/238 (72%)	171 (99%)	1 (1%)	0	100 100
1	G	187/238 (79%)	185 (99%)	1 (0%)	1 (0%)	34 30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	160/238 (67%)	159 (99%)	1 (1%)	0	100 100
All	All	1441/1904 (76%)	1411 (98%)	23 (2%)	7 (0%)	34 30

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	C	196	GLY
1	A	197	ASN
1	E	197	ASN
1	G	197	ASN
1	C	166	SER
1	B	131	GLY

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	168/191 (88%)	164 (98%)	4 (2%)	57 61
1	B	144/191 (75%)	142 (99%)	2 (1%)	74 80
1	C	162/191 (85%)	156 (96%)	6 (4%)	41 41
1	D	139/191 (73%)	135 (97%)	4 (3%)	50 53
1	E	168/191 (88%)	165 (98%)	3 (2%)	66 72
1	F	145/191 (76%)	142 (98%)	3 (2%)	61 66
1	G	161/191 (84%)	155 (96%)	6 (4%)	41 41
1	H	140/191 (73%)	137 (98%)	3 (2%)	61 66
All	All	1227/1528 (80%)	1196 (98%)	31 (2%)	60 59

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	132	THR
1	A	152	LEU
1	A	195	GLN
1	B	96	TYR
1	B	140	LEU
1	C	30	ARG
1	C	74[A]	LYS
1	C	74[B]	LYS
1	C	96	TYR
1	C	142	GLN
1	C	189	ILE
1	D	96	TYR
1	D	157	ARG
1	D	172	GLU
1	D	173	ARG
1	E	96	TYR
1	E	157	ARG
1	E	168	ILE
1	F	96[A]	TYR
1	F	96[B]	TYR
1	F	138	MET
1	G	7[A]	ARG
1	G	7[B]	ARG
1	G	96	TYR
1	G	134	ILE
1	G	173	ARG
1	G	202	LEU
1	H	32	SER
1	H	96[A]	TYR
1	H	96[B]	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	GLN
1	C	211	GLN
1	E	142	GLN
1	E	195	GLN
1	G	142	GLN
1	G	158	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

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	205/238 (86%)	0.94	37 (18%)	2 2	14, 40, 86, 96	0
1	B	175/238 (73%)	0.97	32 (18%)	2 2	15, 38, 70, 86	0
1	C	193/238 (81%)	0.93	26 (13%)	4 6	18, 49, 78, 92	0
1	D	170/238 (71%)	0.92	22 (12%)	5 6	16, 41, 74, 87	0
1	E	205/238 (86%)	1.00	36 (17%)	2 3	19, 41, 84, 95	0
1	F	177/238 (74%)	0.96	31 (17%)	2 3	17, 39, 76, 96	0
1	G	194/238 (81%)	0.92	32 (16%)	2 3	20, 50, 79, 93	0
1	H	169/238 (71%)	0.86	26 (15%)	3 4	19, 41, 66, 84	0
All	All	1488/1904 (78%)	0.94	242 (16%)	2 3	14, 43, 80, 96	0

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	30	ARG	9.2
1	B	1	MET	8.7
1	F	27	LYS	8.2
1	A	162	LYS	8.1
1	E	214	ILE	7.4
1	F	30	ARG	7.4
1	F	173	ARG	6.7
1	A	27	LYS	6.3
1	G	161	GLY	6.2
1	E	210	ALA	6.1
1	E	162	LYS	6.1
1	E	164	GLU	6.1
1	E	197	ASN	6.0
1	C	129	THR	5.9
1	D	168	ILE	5.7
1	B	26	LEU	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	199	THR	5.5
1	E	132	THR	5.4
1	A	214	ILE	5.3
1	B	130	ALA	5.3
1	C	25	THR	5.2
1	G	133	ALA	5.1
1	A	210	ALA	5.0
1	C	165	LEU	4.9
1	D	25	THR	4.8
1	E	27	LYS	4.8
1	D	29	GLY	4.8
1	F	26	LEU	4.8
1	H	31	LYS	4.7
1	F	155	ILE	4.7
1	D	31	LYS	4.7
1	C	167	ALA	4.7
1	E	163	GLY	4.6
1	F	158	GLN	4.6
1	H	168	ILE	4.6
1	F	154	ALA	4.5
1	A	129	THR	4.5
1	F	28	SER	4.5
1	G	197	ASN	4.4
1	A	197	ASN	4.4
1	C	111	ASN	4.4
1	E	161	GLY	4.3
1	A	130	ALA	4.3
1	B	30	ARG	4.3
1	B	153	VAL	4.3
1	B	173	ARG	4.2
1	B	27	LYS	4.1
1	A	196	GLY	4.1
1	A	164	GLU	4.1
1	G	31	LYS	4.1
1	H	25	THR	4.1
1	B	170	GLU	4.1
1	A	211	GLN	4.1
1	C	160	LYS	4.0
1	G	189	ILE	4.0
1	D	173	ARG	3.9
1	A	28	SER	3.9
1	F	78	ILE	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	132	THR	3.8
1	H	111	ASN	3.8
1	G	194	GLN	3.7
1	E	111	ASN	3.7
1	B	78	ILE	3.7
1	E	25	THR	3.7
1	A	163	GLY	3.7
1	A	24	PHE	3.6
1	G	199	THR	3.6
1	A	102	GLU	3.6
1	F	79	ALA	3.6
1	C	3	LYS	3.6
1	F	29	GLY	3.5
1	B	79	ALA	3.5
1	B	167	ALA	3.5
1	E	78	ILE	3.5
1	E	139	GLU	3.5
1	B	154	ALA	3.4
1	D	158	GLN	3.4
1	B	172	GLU	3.4
1	F	25	THR	3.4
1	G	129	THR	3.3
1	E	129	THR	3.3
1	E	102	GLU	3.3
1	G	136	GLU	3.3
1	E	199	THR	3.3
1	H	155	ILE	3.2
1	B	155	ILE	3.2
1	E	28	SER	3.2
1	H	145	LYS	3.2
1	C	30	ARG	3.2
1	H	173	ARG	3.2
1	E	130	ALA	3.2
1	D	101	LYS	3.1
1	D	129	THR	3.1
1	H	101	LYS	3.1
1	H	169	GLN	3.1
1	A	194	GLN	3.1
1	A	143	ALA	3.1
1	B	82	THR	3.1
1	H	158	GLN	3.1
1	C	78	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	170	GLU	3.0
1	D	78	ILE	3.0
1	A	207	ALA	3.0
1	A	78	ILE	3.0
1	H	80	THR	3.0
1	H	124	VAL	3.0
1	B	31	LYS	3.0
1	D	169	GLN	3.0
1	E	22	GLY	2.9
1	G	141	ILE	2.9
1	E	212	TYR	2.9
1	B	124	VAL	2.9
1	C	24	PHE	2.9
1	G	25	THR	2.9
1	G	78	ILE	2.9
1	C	142	GLN	2.9
1	F	169	GLN	2.9
1	C	197	ASN	2.9
1	G	82	THR	2.9
1	A	200	GLU	2.9
1	G	214	ILE	2.9
1	F	50	LEU	2.8
1	F	130	ALA	2.8
1	F	168	ILE	2.8
1	A	111	ASN	2.8
1	E	24	PHE	2.8
1	A	79	ALA	2.8
1	E	81	THR	2.8
1	E	196	GLY	2.8
1	H	123	LEU	2.8
1	A	133	ALA	2.8
1	H	79	ALA	2.7
1	C	198	ASN	2.7
1	G	160	LYS	2.7
1	E	200	GLU	2.7
1	G	178	ALA	2.7
1	G	111	ASN	2.7
1	G	145	LYS	2.7
1	D	124	VAL	2.7
1	F	80	THR	2.7
1	F	82	THR	2.7
1	H	167	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	152	LEU	2.6
1	C	214	ILE	2.6
1	H	96[A]	TYR	2.6
1	F	152	LEU	2.6
1	F	143	ALA	2.6
1	A	29	GLY	2.6
1	G	24	PHE	2.6
1	D	194	GLN	2.6
1	F	84	VAL	2.6
1	D	116	LYS	2.6
1	F	54	TYR	2.6
1	G	166	SER	2.6
1	H	116	LYS	2.6
1	D	80	THR	2.5
1	C	124	VAL	2.5
1	G	35	PHE	2.5
1	F	167	ALA	2.5
1	A	26	LEU	2.5
1	B	152	LEU	2.5
1	E	203	GLU	2.5
1	H	81	THR	2.5
1	C	116	LYS	2.5
1	G	26	LEU	2.5
1	C	196	GLY	2.5
1	E	213	GLY	2.5
1	F	68	LEU	2.5
1	B	77	PRO	2.4
1	D	145	LYS	2.4
1	C	84	VAL	2.4
1	E	51	GLY	2.4
1	A	25	THR	2.4
1	E	76	ILE	2.4
1	G	144	ASN	2.4
1	A	161	GLY	2.4
1	B	51	GLY	2.4
1	B	84	VAL	2.4
1	B	169	GLN	2.4
1	B	25	THR	2.4
1	E	165	LEU	2.4
1	A	203	GLU	2.4
1	G	79	ALA	2.3
1	A	183	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	80	THR	2.3
1	C	194	GLN	2.3
1	E	85	ALA	2.3
1	G	77	PRO	2.3
1	D	79	ALA	2.3
1	C	54	TYR	2.3
1	C	26	LEU	2.3
1	G	198	ASN	2.3
1	A	136	GLU	2.2
1	F	83	ALA	2.2
1	H	154	ALA	2.2
1	E	124	VAL	2.2
1	F	124	VAL	2.2
1	C	141	ILE	2.2
1	B	38	ALA	2.2
1	D	152	LEU	2.2
1	H	84	VAL	2.2
1	F	31	LYS	2.2
1	B	76	ILE	2.2
1	H	78	ILE	2.2
1	E	48	ALA	2.2
1	H	174	ASP	2.2
1	B	123	LEU	2.2
1	B	81	THR	2.2
1	H	82	THR	2.2
1	C	210	ALA	2.2
1	A	165	LEU	2.2
1	E	75	GLY	2.2
1	A	139	GLU	2.2
1	H	3	LYS	2.2
1	G	116	LYS	2.1
1	A	198	ASN	2.1
1	D	77	PRO	2.1
1	G	76	ILE	2.1
1	B	132	THR	2.1
1	B	83	ALA	2.1
1	C	23	GLU	2.1
1	D	84	VAL	2.1
1	A	81	THR	2.1
1	A	213	GLY	2.1
1	E	29	GLY	2.1
1	G	48	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	23	GLU	2.1
1	C	145	LYS	2.1
1	F	77	PRO	2.1
1	A	47	LEU	2.0
1	D	175	PHE	2.0
1	F	81	THR	2.0
1	G	80	THR	2.0
1	B	182	ILE	2.0
1	C	152	LEU	2.0
1	B	102	GLU	2.0
1	G	170	GLU	2.0
1	E	80	THR	2.0
1	E	211	GLN	2.0
1	D	54	TYR	2.0
1	F	75	GLY	2.0
1	G	51	GLY	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	CL	H	216	1/1	0.90	0.17	-0.05	61,61,61,61	0
2	CL	H	215	1/1	0.91	0.11	-	62,62,62,62	0
2	CL	A	215	1/1	0.98	0.08	-	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.