



Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 04:52 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.; Dubrovskaya, 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 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/ValidationPDFNotes.html>

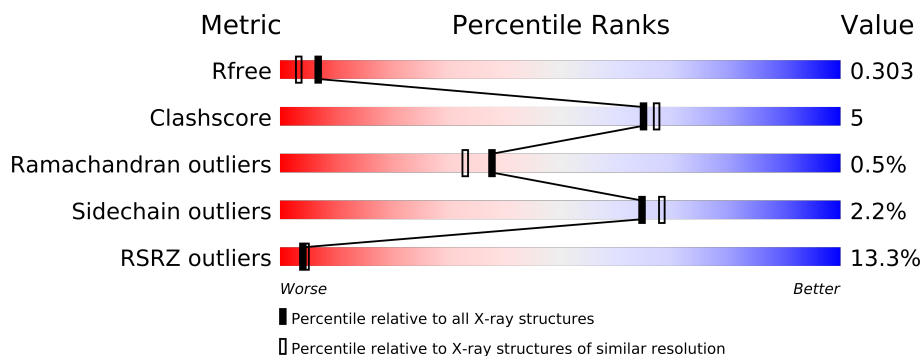
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	238	
1	B	238	
1	C	238	
1	D	238	
1	E	238	
1	F	238	
1	G	238	
1	H	238	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12436 atoms, of which 0 are hydrogen and 0 are deuterium.

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 74	O 74	0	1
3	H	71	Total 72	O 72	0	1

4 Data and refinement statistics

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) 99.6 (29.66-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.222 , 0.269 0.265 , 0.303	Depositor DCC
R_{free} test set	5712 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 , 27.5	EDS
Estimated twinning fraction	0.052 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

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(°)	Ideal(°)
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(°)	Ideal(°)
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 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1626	0	0	13	0
1	B	1377	0	0	5	0
1	C	1546	0	0	15	0
1	D	1330	0	0	3	0
1	E	1626	0	0	12	0
1	F	1391	0	0	4	0
1	G	1554	0	0	9	0
1	H	1335	0	0	4	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	1	0
3	C	79	0	0	5	0
3	D	74	0	0	1	0
3	E	101	0	0	5	0
3	F	69	0	0	0	0
3	G	74	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	72	0	0	2	0
All	All	12436	0	0	63	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (63) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:99:ASN:ND2	3:G:532:HOH:O	2.20	0.74
1:G:140:LEU:O	1:G:144:ASN:ND2	2.21	0.73
1:C:140:LEU:O	1:C:144:ASN:ND2	2.25	0.68
1:A:201:HIS:NE2	3:A:578:HOH:O	2.26	0.68
1:B:101:LYS:O	1:B:102:GLU:C	2.32	0.66
1:E:45:ARG:NH1	3:E:596:HOH:O	2.28	0.66
1:C:69:PHE:CD1	1:C:97[B]:CYS:SG	2.90	0.65
1:E:15:GLU:OE1	1:E:49:ARG:NH2	2.32	0.63
1:A:140:LEU:O	1:A:144:ASN:ND2	2.32	0.63
1:D:25:THR:C	1:D:30:ARG:O	2.38	0.62
1:C:74[A]:LYS:NZ	3:C:233:HOH:O	2.34	0.61
1:C:195:GLN:O	1:C:196:GLY:O	2.19	0.60
1:A:196:GLY:O	1:A:197:ASN:C	2.40	0.60
1:E:209:ARG:O	1:E:213:GLY:N	2.37	0.58
1:A:7:ARG:NH2	3:A:498:HOH:O	2.38	0.57
1:C:173:ARG:NH2	1:C:174:ASP:OD1	2.37	0.57
1:A:45[B]:ARG:NE	3:A:218:HOH:O	2.36	0.57
1:H:158:GLN:NE2	3:H:239:HOH:O	2.37	0.57
1:E:101:LYS:O	1:E:102:GLU:C	2.44	0.56
1:C:30:ARG:NH2	1:C:159:GLU:OE1	2.39	0.55
1:C:209:ARG:O	1:C:213:GLY:N	2.40	0.55
1:B:140:LEU:O	1:B:144:ASN:ND2	2.41	0.53
1:A:100:ARG:NH1	2:A:215:CL:CL	2.79	0.52
1:B:74:LYS:NZ	1:B:126:ASP:OD2	2.43	0.52
1:G:202:LEU:CD2	1:G:202:LEU:C	2.78	0.52
1:G:16:LYS:NZ	3:G:304:HOH:O	2.43	0.52
1:C:45:ARG:NH2	3:C:595:HOH:O	2.44	0.50
1:E:52:ARG:NE	3:E:284:HOH:O	2.45	0.50
1:E:161:GLY:O	1:E:162:LYS:C	2.48	0.49
1:A:45[B]:ARG:NH1	3:A:246:HOH:O	2.46	0.49
1:A:152:LEU:CD2	1:A:153:VAL:O	2.61	0.48
1:G:20:LYS:NZ	3:G:219:HOH:O	2.47	0.48
1:D:157:ARG:NH1	3:D:314:HOH:O	2.46	0.48
1:A:209:ARG:O	1:A:213:GLY:N	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:198:ASN:O	1:C:202:LEU:N	2.47	0.47
1:E:7:ARG:NE	3:E:224:HOH:O	2.47	0.47
1:H:145:LYS:CG	1:H:145:LYS:O	2.63	0.47
1:A:101:LYS:O	1:A:102:GLU:CG	2.63	0.47
1:C:100:ARG:NH1	3:C:222:HOH:O	2.47	0.47
1:D:128:ILE:O	1:D:129:THR:OG1	2.32	0.47
1:E:100:ARG:NH1	3:E:644:HOH:O	2.47	0.47
1:F:157:ARG:O	1:F:158:GLN:CB	2.64	0.46
1:H:120:ARG:NH2	3:H:538:HOH:O	2.48	0.46
1:C:99:ASN:ND2	3:C:452:HOH:O	2.49	0.46
1:A:151:VAL:O	1:A:180:ILE:N	2.50	0.45
1:C:120:ARG:NH1	3:C:469:HOH:O	2.49	0.45
1:E:88:ASP:OD2	1:F:52:ARG:NH1	2.50	0.45
1:E:126:ASP:OD1	1:E:127:VAL:N	2.49	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:24:PHE:O	1:A:32:SER:N	2.50	0.44
1:C:202:LEU:CD2	1:C:202:LEU:C	2.86	0.44
1:G:30:ARG:NH2	3:G:228:HOH:O	2.50	0.44
1:G:16:LYS:O	1:G:17:GLN:CB	2.66	0.43
1:G:66:ASP:OD2	1:G:120:ARG:N	2.51	0.43
1:A:214:ILE:N	1:A:214:ILE:CD1	2.81	0.43
1:C:12:PHE:CE2	1:C:41:PHE:CE1	3.08	0.42
1:E:209:ARG:NH1	3:E:493:HOH:O	2.51	0.42
1:F:15:GLU:OE2	1:F:16:LYS:NZ	2.53	0.41
1:E:196:GLY:O	1:E:197:ASN:C	2.59	0.41
1:B:145:LYS:NZ	3:B:230:HOH:O	2.54	0.41
1:F:24:PHE:O	1:F:32:SER:N	2.54	0.40
1:C:126:ASP:OD1	1:C:127:VAL:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	204/238 (86%)	197 (97%)	5 (2%)	2 (1%)	22	14
1	B	168/238 (71%)	164 (98%)	3 (2%)	1 (1%)	33	28
1	C	186/238 (78%)	182 (98%)	2 (1%)	2 (1%)	21	13
1	D	160/238 (67%)	157 (98%)	3 (2%)	0	100	100
1	E	204/238 (86%)	196 (96%)	7 (3%)	1 (0%)	38	33
1	F	172/238 (72%)	171 (99%)	1 (1%)	0	100	100
1	G	187/238 (79%)	185 (99%)	1 (0%)	1 (0%)	38	33
1	H	160/238 (67%)	159 (99%)	1 (1%)	0	100	100
All	All	1441/1904 (76%)	1411 (98%)	23 (2%)	7 (0%)	38	33

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 ⓘ

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%)	61	65
1	B	144/191 (75%)	142 (99%)	2 (1%)	78	83
1	C	162/191 (85%)	156 (96%)	6 (4%)	45	45
1	D	139/191 (73%)	135 (97%)	4 (3%)	55	57
1	E	168/191 (88%)	165 (98%)	3 (2%)	71	75
1	F	145/191 (76%)	142 (98%)	3 (2%)	66	70
1	G	161/191 (84%)	155 (96%)	6 (4%)	45	45
1	H	140/191 (73%)	137 (98%)	3 (2%)	66	70

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1227/1528 (80%)	1196 (98%)	31 (2%)	64 63

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

Mol	Chain	Res	Type
1	A	96	TYR
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. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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.

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, 95th 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%)	0.84	30 (14%) 3 3	14, 40, 86, 96	0
1	B	175/238 (73%)	0.90	22 (12%) 4 5	15, 38, 70, 86	0
1	C	193/238 (81%)	0.87	21 (10%) 6 7	18, 49, 78, 92	0
1	D	170/238 (71%)	0.81	15 (8%) 10 11	16, 41, 74, 87	0
1	E	205/238 (86%)	0.92	32 (15%) 3 3	19, 41, 84, 95	0
1	F	177/238 (74%)	0.87	23 (12%) 4 5	17, 39, 76, 96	0
1	G	194/238 (81%)	0.85	31 (15%) 3 3	20, 50, 79, 93	0
1	H	169/238 (71%)	0.79	24 (14%) 3 4	19, 41, 66, 84	0
All	All	1488/1904 (78%)	0.86	198 (13%) 4 4	14, 43, 80, 96	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	162	LYS	8.5
1	E	214	ILE	8.2
1	D	30	ARG	8.1
1	F	30	ARG	7.7
1	F	27	LYS	7.6
1	F	173	ARG	6.7
1	E	162	LYS	6.5
1	B	1	MET	6.2
1	E	164	GLU	6.0
1	A	214	ILE	5.8
1	B	26	LEU	5.7
1	A	27	LYS	5.7
1	E	197	ASN	5.6
1	D	31	LYS	5.4
1	C	25	THR	5.4
1	C	129	THR	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	130	ALA	5.2
1	E	210	ALA	5.1
1	D	168	ILE	5.1
1	H	31	LYS	5.1
1	G	161	GLY	5.0
1	D	29	GLY	5.0
1	A	199	THR	4.9
1	F	26	LEU	4.9
1	E	161	GLY	4.8
1	F	28	SER	4.7
1	E	132	THR	4.6
1	E	163	GLY	4.6
1	A	164	GLU	4.6
1	C	167	ALA	4.5
1	H	168	ILE	4.5
1	F	155	ILE	4.5
1	E	27	LYS	4.4
1	A	196	GLY	4.3
1	F	154	ALA	4.3
1	D	25	THR	4.3
1	B	153	VAL	4.2
1	C	160	LYS	4.2
1	B	173	ARG	4.2
1	B	30	ARG	4.1
1	G	31	LYS	4.1
1	A	28	SER	4.1
1	B	170	GLU	4.1
1	A	129	THR	4.1
1	H	25	THR	4.1
1	G	197	ASN	4.0
1	H	169	GLN	3.9
1	F	29	GLY	3.9
1	A	197	ASN	3.9
1	C	196	GLY	3.9
1	D	173	ARG	3.8
1	C	165	LEU	3.8
1	F	158	GLN	3.7
1	B	27	LYS	3.7
1	A	210	ALA	3.7
1	G	194	GLN	3.6
1	G	189	ILE	3.6
1	D	169	GLN	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	133	ALA	3.6
1	F	78	ILE	3.6
1	C	111	ASN	3.5
1	H	132	THR	3.5
1	B	172	GLU	3.5
1	C	3	LYS	3.5
1	A	211	GLN	3.5
1	G	136	GLU	3.5
1	A	102	GLU	3.5
1	B	167	ALA	3.4
1	A	163	GLY	3.4
1	G	166	SER	3.4
1	B	79	ALA	3.4
1	B	78	ILE	3.4
1	F	79	ALA	3.4
1	A	24	PHE	3.4
1	A	130	ALA	3.3
1	E	129	THR	3.3
1	A	143	ALA	3.2
1	E	102	GLU	3.2
1	F	25	THR	3.2
1	B	154	ALA	3.2
1	F	168	ILE	3.1
1	H	111	ASN	3.1
1	F	170	GLU	3.1
1	H	173	ARG	3.1
1	F	169	GLN	3.0
1	D	158	GLN	3.0
1	E	196	GLY	3.0
1	H	145	LYS	3.0
1	A	200	GLU	3.0
1	E	139	GLU	3.0
1	E	111	ASN	3.0
1	H	158	GLN	3.0
1	G	178	ALA	3.0
1	B	82	THR	2.9
1	C	214	ILE	2.9
1	E	78	ILE	2.9
1	G	214	ILE	2.9
1	G	199	THR	2.9
1	E	212	TYR	2.9
1	B	155	ILE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	28	SER	2.8
1	C	30	ARG	2.8
1	H	155	ILE	2.8
1	H	116	LYS	2.8
1	G	82	THR	2.8
1	H	79	ALA	2.8
1	G	129	THR	2.7
1	C	194	GLN	2.7
1	A	26	LEU	2.7
1	G	26	LEU	2.7
1	D	194	GLN	2.7
1	B	124	VAL	2.7
1	E	25	THR	2.7
1	G	25	THR	2.7
1	C	116	LYS	2.7
1	C	78	ILE	2.6
1	E	203	GLU	2.6
1	B	25	THR	2.6
1	G	144	ASN	2.6
1	A	194	GLN	2.6
1	H	124	VAL	2.6
1	A	111	ASN	2.6
1	H	133	ALA	2.6
1	D	78	ILE	2.6
1	G	145	LYS	2.6
1	A	203	GLU	2.5
1	B	169	GLN	2.5
1	E	22	GLY	2.5
1	A	133	ALA	2.5
1	H	123	LEU	2.5
1	E	51	GLY	2.5
1	G	78	ILE	2.5
1	B	51	GLY	2.5
1	E	213	GLY	2.5
1	G	35	PHE	2.5
1	F	130	ALA	2.5
1	H	167	ALA	2.5
1	C	124	VAL	2.5
1	F	82	THR	2.4
1	D	129	THR	2.4
1	E	81	THR	2.4
1	C	142	GLN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	76	ILE	2.4
1	D	116	LYS	2.4
1	C	24	PHE	2.4
1	A	165	LEU	2.4
1	F	50	LEU	2.4
1	B	31	LYS	2.4
1	G	160	LYS	2.4
1	H	101	LYS	2.4
1	G	141	ILE	2.4
1	C	26	LEU	2.3
1	H	152	LEU	2.3
1	C	84	VAL	2.3
1	D	145	LYS	2.3
1	C	197	ASN	2.3
1	A	29	GLY	2.3
1	E	24	PHE	2.3
1	A	79	ALA	2.3
1	A	78	ILE	2.3
1	E	165	LEU	2.3
1	H	80	THR	2.3
1	D	79	ALA	2.3
1	G	79	ALA	2.3
1	B	182	ILE	2.3
1	G	196	GLY	2.3
1	E	199	THR	2.3
1	E	23	GLU	2.2
1	A	183	VAL	2.2
1	G	111	ASN	2.2
1	H	82	THR	2.2
1	C	152	LEU	2.2
1	A	161	GLY	2.2
1	H	96[A]	TYR	2.2
1	F	83	ALA	2.2
1	C	203	GLU	2.2
1	E	200	GLU	2.2
1	G	139	GLU	2.2
1	G	24	PHE	2.1
1	G	76	ILE	2.1
1	D	124	VAL	2.1
1	G	64	GLU	2.1
1	F	152	LEU	2.1
1	E	75	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	48	ALA	2.1
1	F	80	THR	2.1
1	H	154	ALA	2.1
1	A	81	THR	2.1
1	H	194	GLN	2.0
1	B	81	THR	2.0
1	F	54	TYR	2.0
1	A	25	THR	2.0
1	E	85	ALA	2.0
1	E	130	ALA	2.0
1	G	116	LYS	2.0
1	H	81	THR	2.0
1	G	170	GLU	2.0
1	F	75	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CL	H	216	1/1	0.17	-0.08	61,61,61,61	0
2	CL	H	215	1/1	0.13	-0.91	62,62,62,62	0
2	CL	A	215	1/1	0.09	-1.88	43,43,43,43	0

6.5 Other polymers ⓘ

There are no such residues in this entry.