



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 09:06 AM GMT

PDB ID : 4ERP
Title : Crystal structure of a gemcitabine-diphosphateinhibited E. coli class Ia ribonucleotide reductase complex
Authors : Zimanyi, C.M.; Drennan, C.L.
Deposited on : 2012-04-20
Resolution : 4.45 Å(reported)

This is a wwPDB validation summary 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>

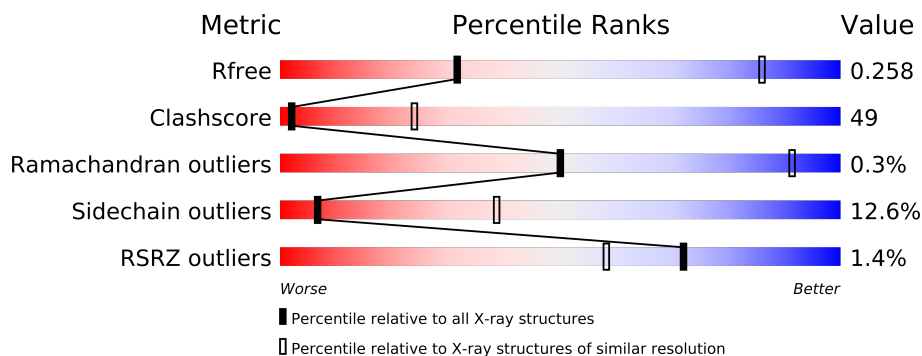
The following versions of software and data (see [references](#)) were used in the production of this report:

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 4.45 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	1020 (5.30-3.50)
Clashscore	79885	1285 (5.30-3.50)
Ramachandran outliers	78287	1214 (5.26-3.50)
Sidechain outliers	78261	1195 (5.26-3.50)
RSRZ outliers	66119	1020 (5.30-3.50)

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	761	
1	B	761	
1	C	761	
1	D	761	
2	E	375	
2	F	375	
2	G	375	
2	H	375	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 35205 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 Ribonucleoside-diphosphatereductase 1 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	734	Total	C	N	O	S	0	0	0
			5845	3712	1004	1105	24			
1	B	735	Total	C	N	O	S	0	0	0
			5850	3715	1005	1106	24			
1	C	733	Total	C	N	O	S	0	0	0
			5841	3710	1003	1104	24			
1	D	736	Total	C	N	O	S	0	0	0
			5859	3720	1007	1108	24			

- Molecule 2 is a protein called Ribonucleoside-diphosphatereductase 1 subunit beta.

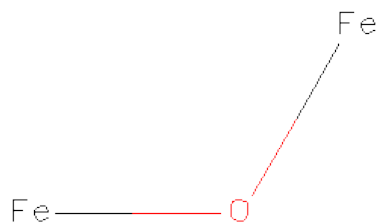
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	354	Total	C	N	O	S	0	0	0
			2900	1850	480	557	13			
2	F	358	Total	C	N	O	S	0	0	0
			2930	1867	486	564	13			
2	G	357	Total	C	N	O	S	0	0	0
			2922	1863	483	563	13			
2	H	356	Total	C	N	O	S	0	0	0
			2914	1857	483	561	13			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is MU-OXO-DIIRON (three-letter code: FEO) (formula: Fe_2O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total 3	Fe 2	O 1	0	0
4	F	1	Total 3	Fe 2	O 1	0	0
4	G	1	Total 3	Fe 2	O 1	0	0
4	H	1	Total 3	Fe 2	O 1	0	0

- Molecule 5 is water.

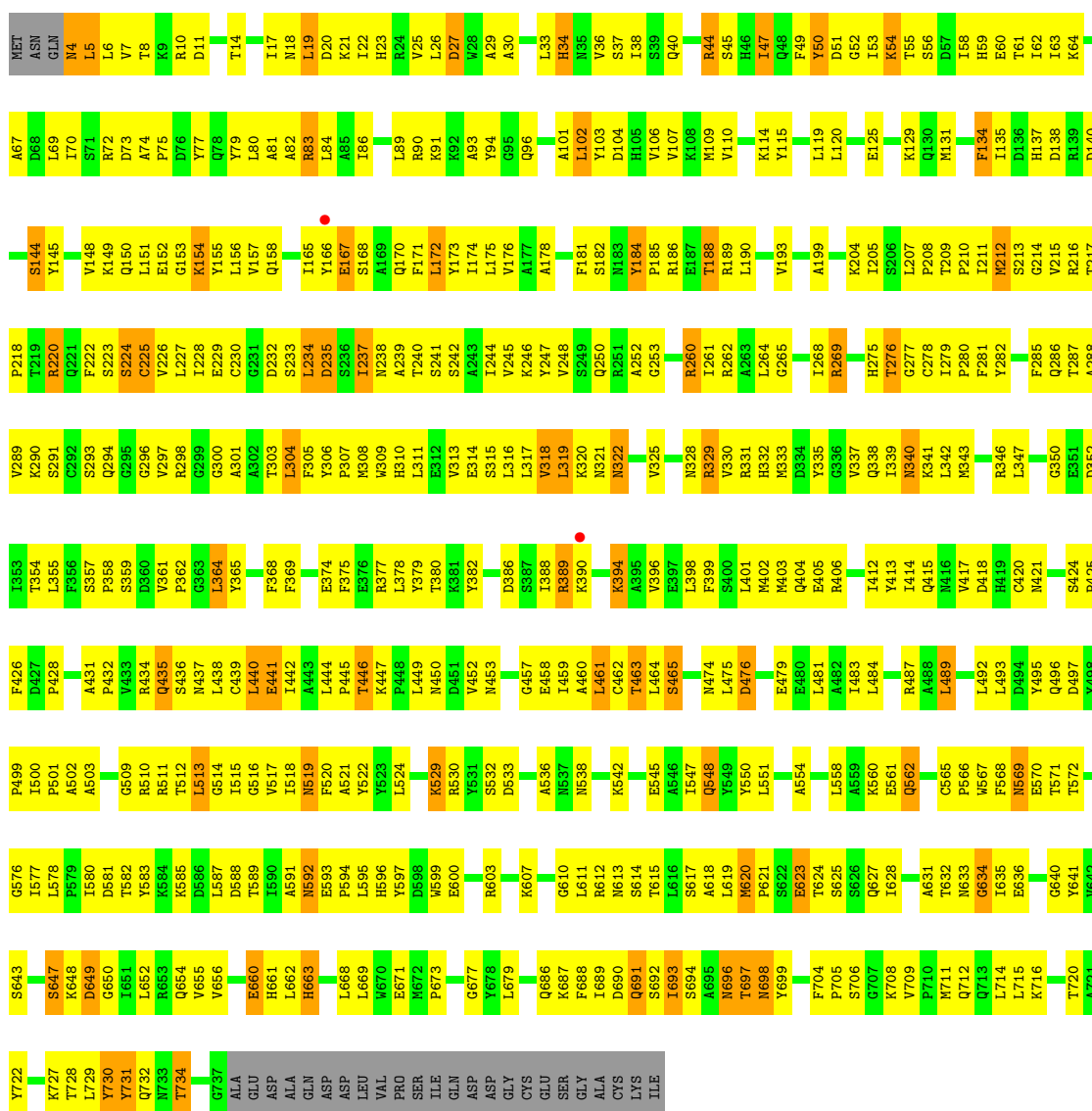
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	2	Total 2	O 2	0	0
5	F	2	Total 2	O 2	0	0
5	G	2	Total 2	O 2	0	0
5	H	2	Total 2	O 2	0	0

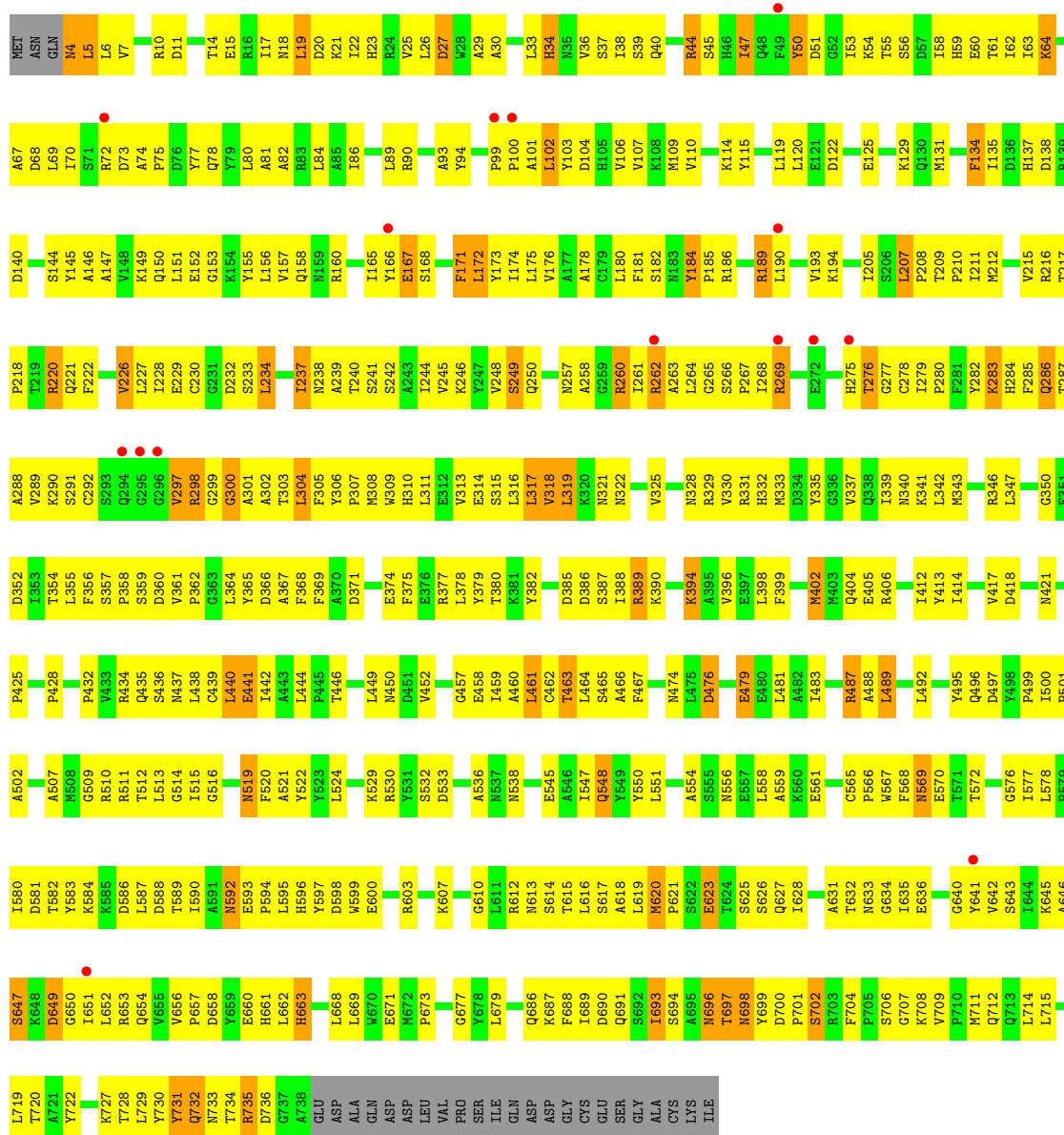
3 Residue-property plots

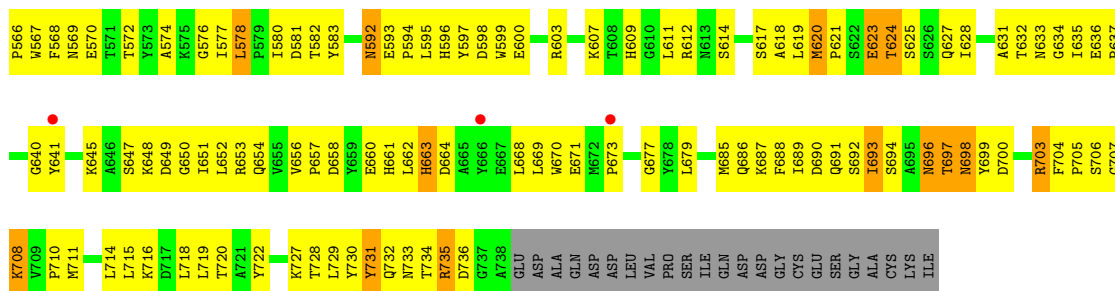
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Ribonucleoside-diphosphatereductase 1 subunit alpha

Chain A:

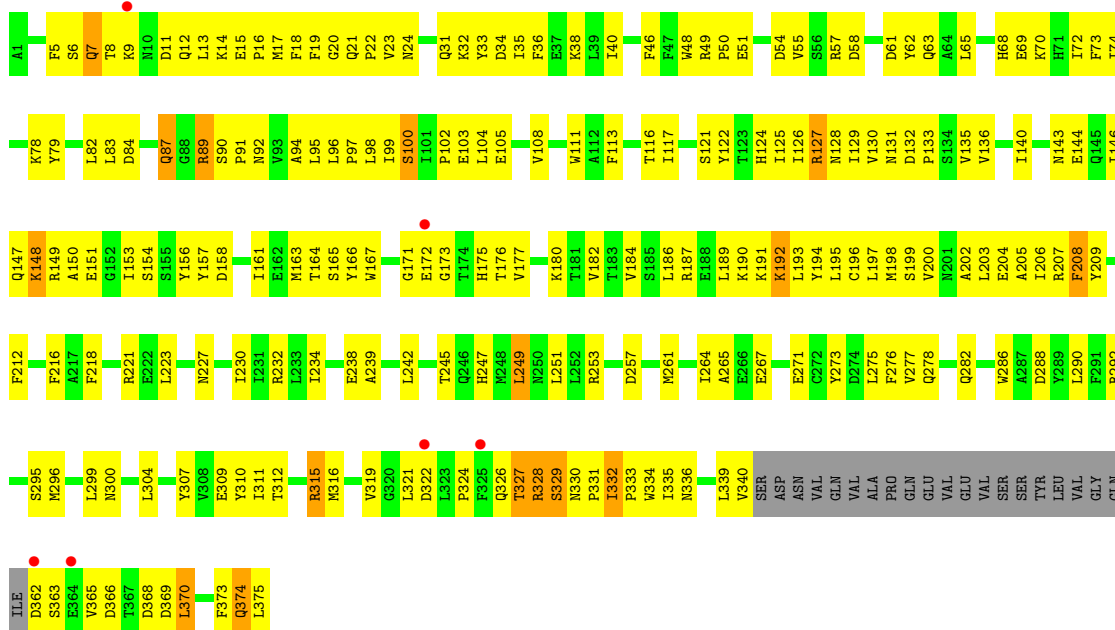






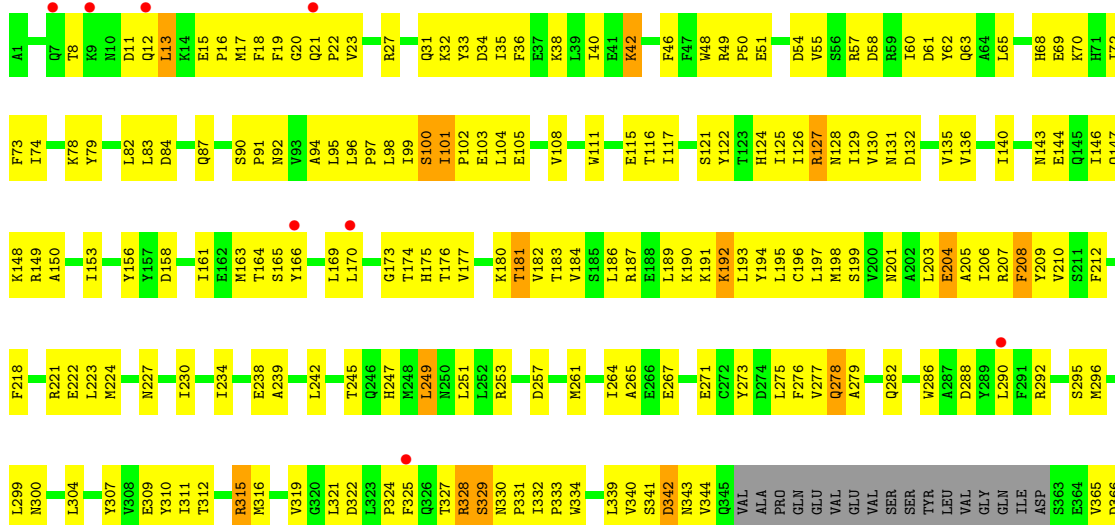
• Molecule 2: Ribonucleoside-diphosphatereductase 1 subunit beta

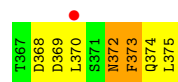
Chain E:



• Molecule 2: Ribonucleoside-diphosphatereductase 1 subunit beta

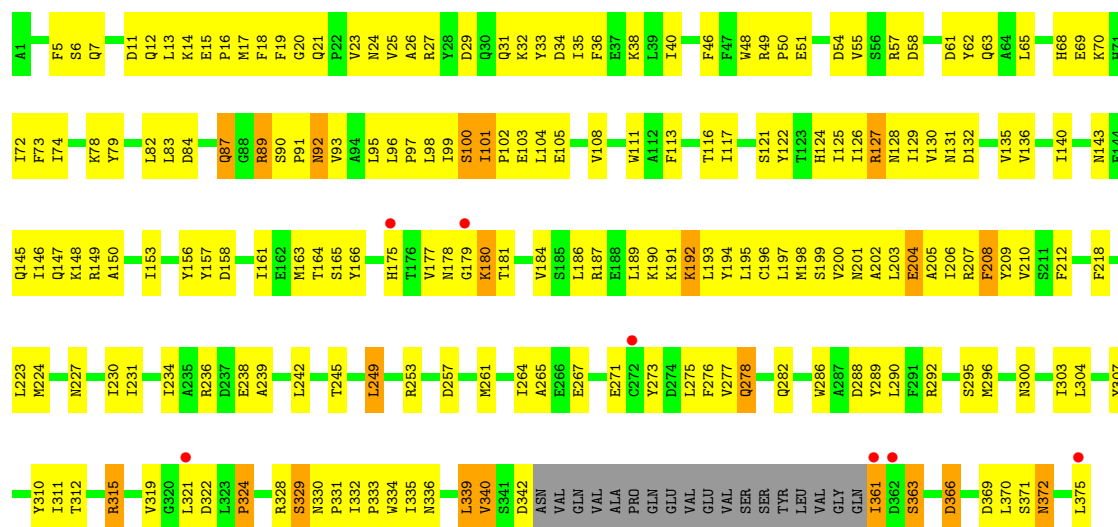
Chain F:





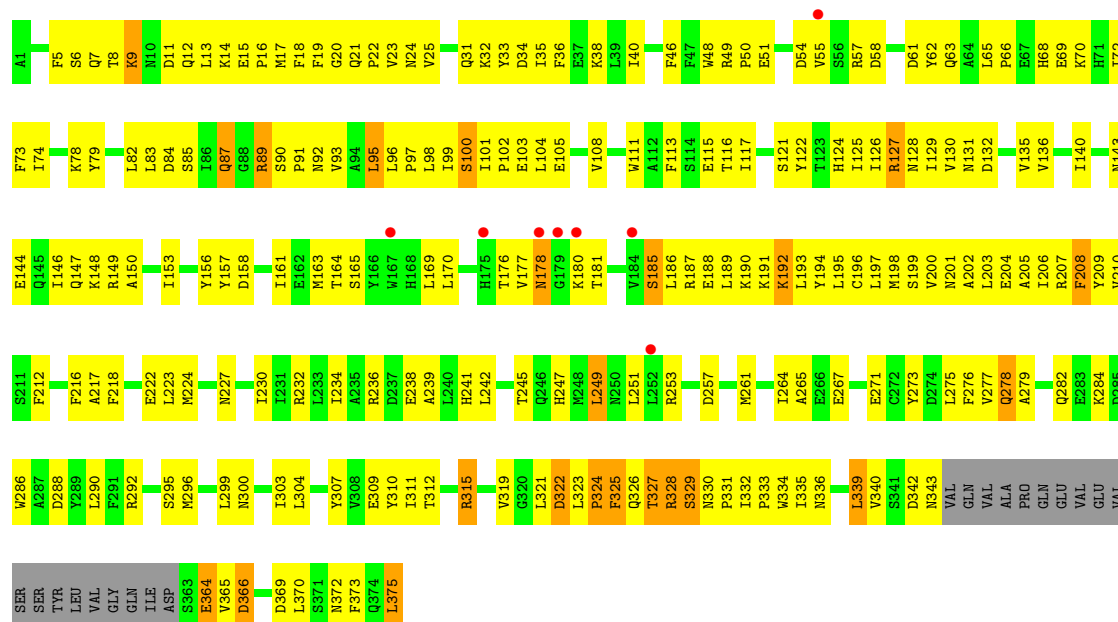
• Molecule 2: Ribonucleoside-diphosphatereductase 1 subunit beta

Chain G:



• Molecule 2: Ribonucleoside-diphosphatereductase 1 subunit beta

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	128.67Å 398.91Å 319.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.45 49.54 – 4.44	Depositor EDS
% Data completeness (in resolution range)	82.3 (50.00-4.45) 81.9 (49.54-4.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 4.45Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.233 , 0.267 0.226 , 0.258	Depositor DCC
R_{free} test set	2128 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	108.8	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 118.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 46097 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	35205	wwPDB-VP
Average B, all atoms (Å ²)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

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: FEO, ATP

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	0.31	0/5973	0.51	0/8090
1	B	0.31	0/5978	0.54	1/8097 (0.0%)
1	C	0.31	0/5969	0.55	0/8085
1	D	0.31	0/5987	0.53	0/8109
2	E	0.32	0/2964	0.49	1/4019 (0.0%)
2	F	0.34	0/2994	0.51	2/4060 (0.0%)
2	G	0.34	0/2986	0.51	2/4049 (0.0%)
2	H	0.33	0/2978	0.48	0/4038
All	All	0.32	0/35829	0.52	6/48547 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	324	PRO	N-CA-C	5.82	127.23	112.10
2	G	92	ASN	N-CA-C	5.57	126.03	111.00
1	B	360	ASP	O-C-N	-5.35	114.14	122.70
2	E	362	ASP	CB-CG-OD2	5.17	122.95	118.30
2	F	342	ASP	CB-CG-OD2	5.14	122.92	118.30

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	5845	0	5770	637	0
1	B	5850	0	5774	647	0
1	C	5841	0	5767	626	0
1	D	5859	0	5783	649	0
2	E	2900	0	2826	238	0
2	F	2930	0	2854	232	0
2	G	2922	0	2846	239	0
2	H	2914	0	2837	275	0
3	A	31	0	12	4	0
3	B	31	0	12	9	0
3	C	31	0	11	15	0
3	D	31	0	12	10	0
4	E	3	0	0	0	0
4	F	3	0	0	0	0
4	G	3	0	0	0	0
4	H	3	0	0	0	0
5	E	2	0	0	1	0
5	F	2	0	0	1	0
5	G	2	0	0	1	0
5	H	2	0	0	0	0
All	All	35205	0	34504	3414	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 49.

The worst 5 of 3414 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:115:TYR:CE1	1:C:216:ARG:HD2	1.42	1.53
1:C:442:ILE:HD12	1:C:462:CYS:SG	1.48	1.51
1:D:114:LYS:HG3	1:D:166:TYR:CE2	1.45	1.50
1:B:222:PHE:CD2	1:B:492:LEU:HD11	1.44	1.49
1:A:5:LEU:HD12	1:A:17:ILE:CG1	1.41	1.49

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	732/761 (96%)	672 (92%)	57 (8%)	3 (0%)	43	90
1	B	733/761 (96%)	679 (93%)	50 (7%)	4 (0%)	38	88
1	C	731/761 (96%)	681 (93%)	48 (7%)	2 (0%)	50	91
1	D	734/761 (96%)	673 (92%)	59 (8%)	2 (0%)	50	91
2	E	350/375 (93%)	325 (93%)	25 (7%)	0	100	100
2	F	354/375 (94%)	326 (92%)	28 (8%)	0	100	100
2	G	353/375 (94%)	328 (93%)	25 (7%)	0	100	100
2	H	352/375 (94%)	327 (93%)	24 (7%)	1 (0%)	50	91
All	All	4339/4544 (96%)	4011 (92%)	316 (7%)	12 (0%)	50	91

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	731	TYR
1	C	731	TYR
1	D	731	TYR
1	B	300	GLY
2	H	324	PRO

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	629/651 (97%)	532 (85%)	97 (15%)	4	28
1	B	629/651 (97%)	545 (87%)	84 (13%)	6	35
1	C	629/651 (97%)	542 (86%)	87 (14%)	5	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	630/651 (97%)	537 (85%)	93 (15%)	4	30
2	E	321/340 (94%)	292 (91%)	29 (9%)	14	56
2	F	325/340 (96%)	297 (91%)	28 (9%)	15	59
2	G	324/340 (95%)	295 (91%)	29 (9%)	14	56
2	H	323/340 (95%)	289 (90%)	34 (10%)	10	48
All	All	3810/3964 (96%)	3329 (87%)	481 (13%)	7	38

5 of 481 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	287	THR
1	D	11	ASP
2	G	366	ASP
1	C	331	ARG
1	C	497	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 123 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	158	GLN
1	C	562	GLN
2	G	227	ASN
1	C	250	GLN
1	C	338	GLN

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

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	ATP	A	801	-	33,33,33	1.98	8 (24%)	52,52,52	2.55	15 (28%)
3	ATP	B	801	-	33,33,33	1.98	8 (24%)	52,52,52	2.55	15 (28%)
3	ATP	C	801	-	33,33,33	1.90	8 (24%)	52,52,52	2.41	16 (30%)
3	ATP	D	801	-	33,33,33	1.95	9 (27%)	52,52,52	2.44	12 (23%)
4	FEO	E	501	2,5	0,2,2	0.00	-	0,1,1	0.00	-
4	FEO	F	501	2,5	0,2,2	0.00	-	0,1,1	0.00	-
4	FEO	G	501	2,5	0,2,2	0.00	-	0,1,1	0.00	-
4	FEO	H	501	2,5	0,2,2	0.00	-	0,1,1	0.00	-

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
3	ATP	A	801	-	-	0/22/38/38	0/1/3/3
3	ATP	B	801	-	-	0/22/38/38	0/1/3/3
3	ATP	C	801	-	-	0/22/38/38	0/1/3/3
3	ATP	D	801	-	-	0/22/38/38	0/1/3/3
4	FEO	E	501	2,5	-	0/0/0/0	0/0/0/0
4	FEO	F	501	2,5	-	0/0/0/0	0/0/0/0
4	FEO	G	501	2,5	-	0/0/0/0	0/0/0/0
4	FEO	H	501	2,5	-	0/0/0/0	0/0/0/0

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	801	ATP	O4'-C1'	4.86	1.48	1.41
3	D	801	ATP	O4'-C1'	4.79	1.48	1.41
3	B	801	ATP	O4'-C1'	4.76	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	ATP	O4'-C1'	4.73	1.48	1.41
3	D	801	ATP	C6-N6	4.68	1.50	1.35

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	ATP	O4'-C1'-N9	10.79	118.47	108.44
3	B	801	ATP	O4'-C1'-N9	10.78	118.47	108.44
3	C	801	ATP	N3-C2-N1	-8.92	121.25	128.71
3	D	801	ATP	O4'-C1'-N9	8.79	116.61	108.44
3	B	801	ATP	N3-C2-N1	-8.71	121.43	128.71

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	734/761 (96%)	0.11	2 (0%) 91 86	62, 120, 165, 251	0
1	B	735/761 (96%)	0.34	15 (2%) 62 49	76, 152, 200, 256	0
1	C	733/761 (96%)	0.17	6 (0%) 83 71	63, 128, 171, 261	0
1	D	736/761 (96%)	0.24	8 (1%) 77 63	68, 133, 187, 253	0
2	E	354/375 (94%)	0.34	6 (1%) 67 54	77, 152, 210, 243	0
2	F	358/375 (95%)	0.45	9 (2%) 54 44	74, 151, 209, 256	0
2	G	357/375 (95%)	0.25	7 (1%) 62 49	96, 162, 207, 255	0
2	H	356/375 (94%)	0.27	8 (2%) 59 47	117, 172, 208, 267	0
All	All	4363/4544 (96%)	0.25	61 (1%) 72 58	62, 141, 198, 267	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	166	TYR	4.4
1	B	295	GLY	3.7
1	C	225	CYS	3.2
1	C	392	ARG	3.1
2	F	9	LYS	3.0

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
3	ATP	C	801	31/31	0.30	0.55	138,138,138,138	0
3	ATP	B	801	31/31	0.46	0.36	225,225,225,225	0
3	ATP	D	801	31/31	0.37	0.15	195,195,195,195	0
3	ATP	A	801	31/31	0.29	-0.27	126,126,126,126	0
4	FEO	F	501	3/3	0.22	-1.03	106,106,106,106	0
4	FEO	G	501	3/3	0.14	-1.50	124,124,124,124	0
4	FEO	H	501	3/3	0.11	-1.84	133,133,133,133	0
4	FEO	E	501	3/3	0.16	-1.96	119,119,119,119	0

6.5 Other polymers

There are no such residues in this entry.