Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:26 AM GMT

PDB ID	:	3ELE
Title	:	Crystal structure of Amino Transferase (RER070207001803) from Eubacterium rectale at 2.10 A resolution
Authors	:	Joint Center for Structural Genomics (JCSG)
Deposited on	:	2008-09-22
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:

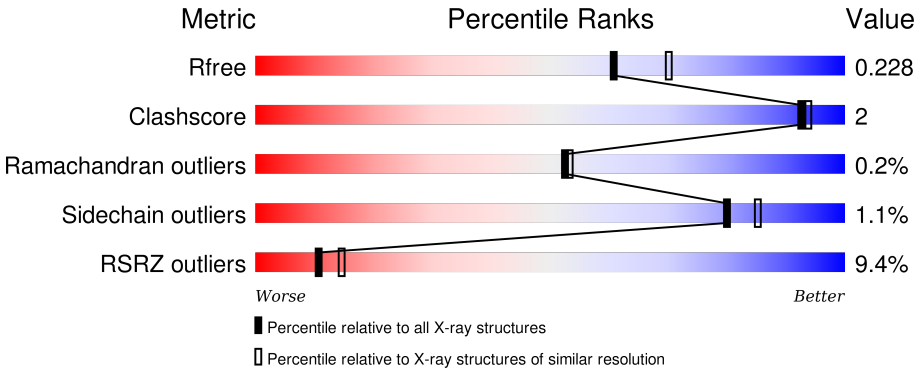
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	398	5% 93% 6%
1	B	398	6% 93% 7%
1	C	398	15% 94% 6%
1	D	398	12% 95% 5%

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
3	EDO	A	502	-	-	-	X
3	EDO	B	503	-	-	-	X
3	EDO	B	504	-	-	-	X
3	EDO	B	508	-	-	-	X

2 Entry composition

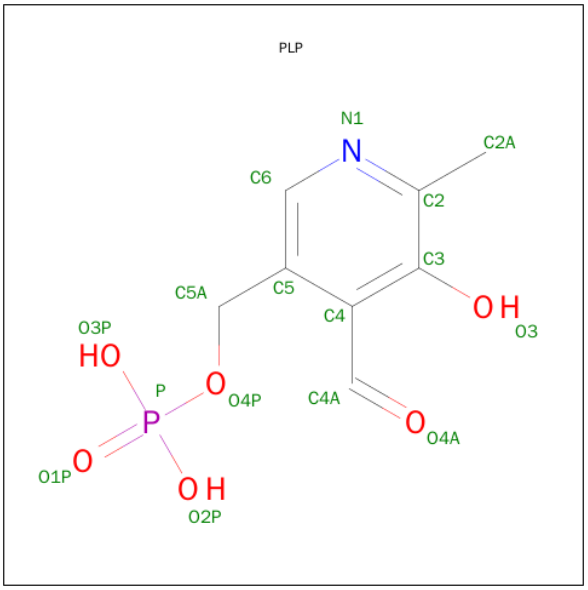
There are 5 unique types of molecules in this entry. The entry contains 13442 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Amino Transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	Se	0	4	0
			3146	2016	513	598	9	10			
1	B	398	Total	C	N	O	S	Se	0	4	0
			3141	2013	507	603	9	9			
1	C	397	Total	C	N	O	S	Se	0	7	0
			3143	2016	509	599	9	10			
1	D	398	Total	C	N	O	S	Se	0	5	0
			3119	2000	501	600	9	9			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

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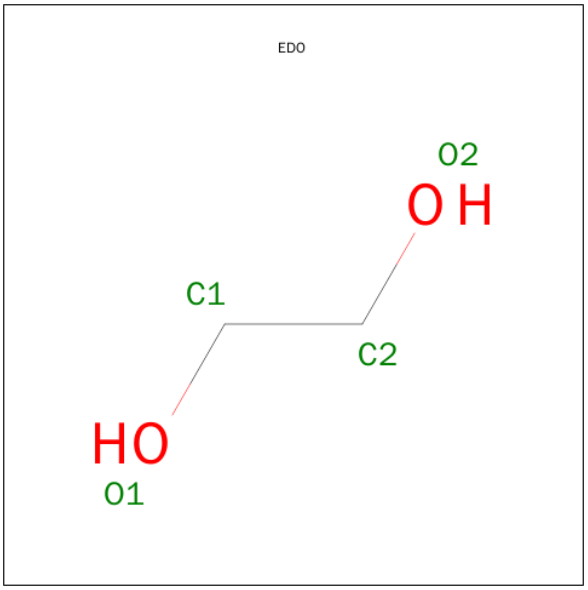
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O P 16 8 1 6 1	0	0
2	D	1	Total C N O P 16 8 1 6 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0

- Molecule 5 is water.

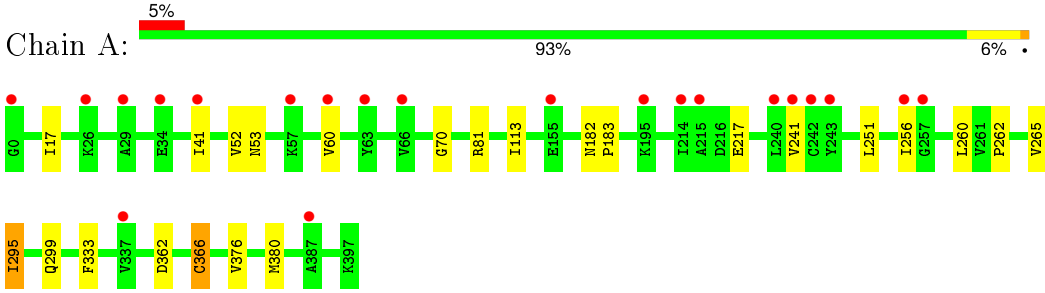
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	501	Total O 506 506	0	5
5	B	113	Total O 113 113	0	0
5	C	83	Total O 85 85	0	2
5	D	75	Total O 75 75	0	0

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.

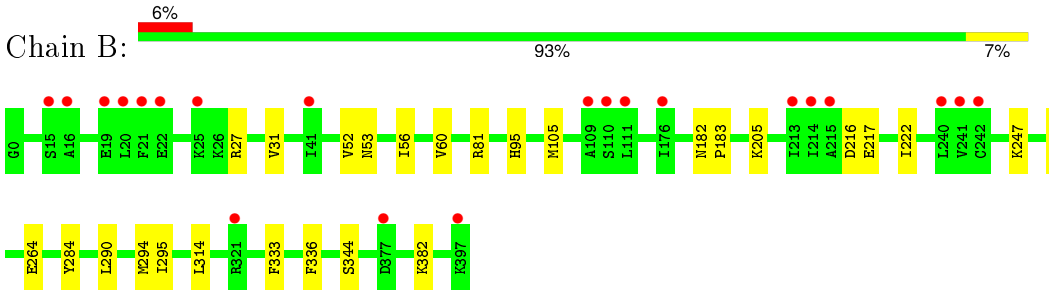
- Molecule 1: Amino Transferase

Chain A:



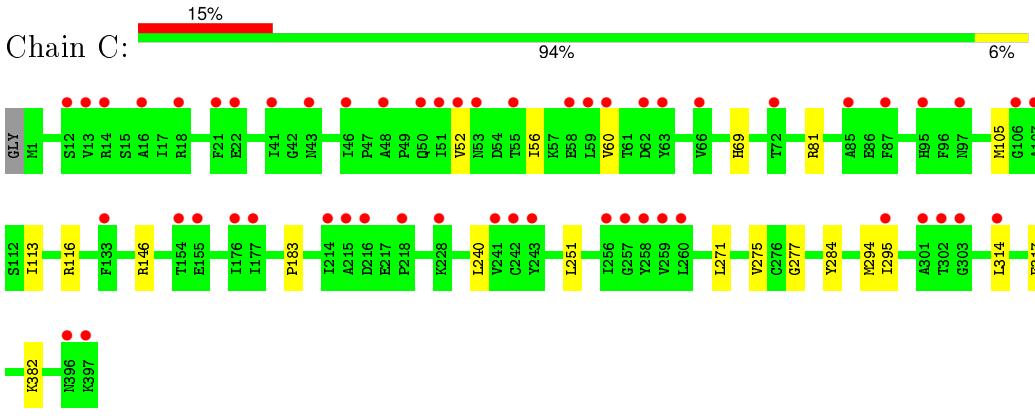
- Molecule 1: Amino Transferase

Chain B:



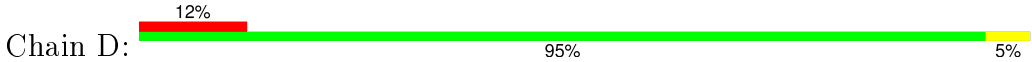
- Molecule 1: Amino Transferase

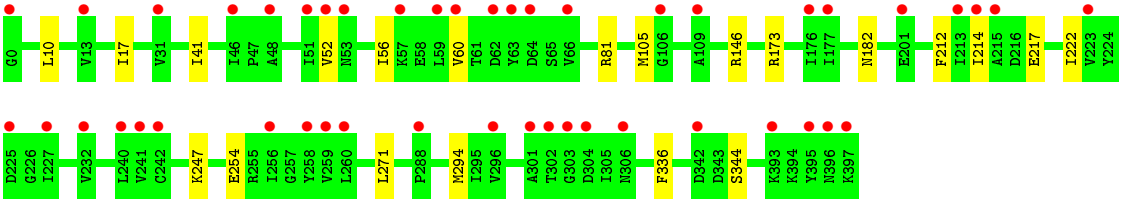
Chain C:



- Molecule 1: Amino Transferase

Chain D:




G0
L10
V13
I17
V31
I41
I46
P47
A48
I51
V52
N53
I56
K57
E58
L59
V60
T61
D62
Y63
D64
S65
V66
R81
M105
G106
A109
R146
R173
I176
I177
N182
E201
F212
I213
I214
A215
D216
E217
I222
V223
Y224
D225
G226
I227
V232
L240
V241
C242
K247
E254
R255
I256
G257
Y258
V259
L260
L271
P288
M294
I295
V296
A301
T302
G303
D304
I305
N306
F336
D342
D343
S344
K393
K394
Y395
N396
K397

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	65.56Å 68.39Å 98.11Å 82.51° 79.52° 75.68°	Depositor
Resolution (Å)	29.88 – 2.10 29.89 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.6 (29.88-2.10) 95.0 (29.89-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.173 , 0.222 0.178 , 0.228	Depositor DCC
R_{free} test set	4610 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	23.6	Xtriage
Anisotropy	0.594	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 92101 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13442	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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: CL, EDO, PLP

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	0.71	1/3222 (0.0%)	0.80	1/4349 (0.0%)
1	B	0.70	0/3217	0.79	1/4345 (0.0%)
1	C	0.67	0/3229	0.80	3/4365 (0.1%)
1	D	0.65	0/3196	0.78	5/4319 (0.1%)
All	All	0.68	1/12864 (0.0%)	0.79	10/17378 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	366	CYS	CB-SG	-5.85	1.72	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	173[A]	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	D	173[B]	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	C	81	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	D	146	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	A	81	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	B	81	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	D	81	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	C	146	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	C	116	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	D	146	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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	3146	0	3087	17	0
1	B	3141	0	3065	18	0
1	C	3143	0	3067	14	0
1	D	3119	0	3027	12	0
2	A	16	0	8	1	0
2	B	16	0	8	2	0
2	C	16	0	8	0	0
2	D	16	0	7	1	0
3	A	8	0	12	0	0
3	B	36	0	54	0	0
3	C	4	0	6	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	506	0	0	0	0
5	B	113	0	0	0	0
5	C	85	0	0	0	0
5	D	75	0	0	0	0
All	All	13442	0	12349	51	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 2.

All (51) 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:D:17:ILE:HG22	1:D:41:ILE:HG22	1.67	0.76
1:B:294[B]:MSE:HE2	1:B:295:ILE:HD12	1.71	0.73
1:C:52:VAL:HG11	1:C:251:LEU:HD21	1.79	0.62
1:B:52:VAL:HG13	1:B:294[B]:MSE:SE	2.50	0.62
1:A:294[B]:MSE:HE2	1:A:295:ILE:HD12	1.82	0.60
1:C:105:MSE:HE2	1:C:284:TYR:CD1	2.38	0.59
1:A:52:VAL:HG13	1:A:294[B]:MSE:SE	2.53	0.58
1:D:52:VAL:HG13	1:D:294[B]:MSE:SE	2.56	0.56
1:A:60:VAL:HG13	1:B:53:ASN:HB3	1.87	0.55
1:C:105:MSE:HE2	1:C:284:TYR:HD1	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:LEU:HD21	1:C:271:LEU:HD21	1.91	0.52
1:A:182:ASN:HB3	2:A:500:PLP:H2A1	1.92	0.51
1:B:182:ASN:HB3	2:B:500:PLP:H2A1	1.93	0.50
1:A:113:ILE:HG21	1:A:275:VAL:HG13	1.93	0.49
1:A:17:ILE:HG22	1:A:41:ILE:HG22	1.95	0.49
1:D:182:ASN:HB3	2:D:500:PLP:H2A1	1.94	0.48
1:B:56:ILE:HG23	1:B:290:LEU:HD21	1.96	0.48
1:A:295:ILE:HG23	1:A:299:GLN:NE2	2.29	0.47
1:C:56:ILE:HG21	1:D:60:VAL:HG21	1.96	0.47
1:D:222:ILE:HD11	1:D:247:LYS:HB3	1.96	0.47
1:C:113:ILE:HG21	1:C:275:VAL:HG13	1.97	0.46
1:C:294[B]:MSE:HE2	1:C:295:ILE:HD12	1.97	0.46
1:C:105:MSE:HE3	1:D:105:MSE:CE	2.45	0.46
1:B:294[B]:MSE:HE2	1:B:295:ILE:CD1	2.45	0.46
1:D:17:ILE:HG22	1:D:41:ILE:CG2	2.40	0.46
1:B:314:LEU:HD21	1:B:382:LYS:HG3	1.98	0.46
1:C:294[B]:MSE:HE2	1:C:295:ILE:CD1	2.46	0.45
1:A:53:ASN:HB3	1:B:60:VAL:HG13	1.99	0.45
1:B:95[A]:HIS:NE2	1:B:264:GLU:OE2	2.48	0.45
1:A:256:ILE:HG12	1:A:295:ILE:HD13	1.99	0.45
1:A:52:VAL:HG11	1:A:251:LEU:HD21	1.98	0.45
1:B:105:MSE:HE2	1:B:284:TYR:CD1	2.51	0.44
1:C:69:HIS:ND1	1:D:254:GLU:OE2	2.51	0.44
1:B:294[A]:MSE:SE	1:B:295:ILE:HD12	2.68	0.43
1:C:60:VAL:HG21	1:D:56:ILE:HG21	1.99	0.43
1:C:314:LEU:HD21	1:C:382:LYS:CG	2.49	0.43
1:A:53:ASN:CB	1:B:60:VAL:HG13	2.49	0.43
1:A:262:PRO:O	1:A:265:VAL:HG22	2.18	0.43
1:B:216:ASP:OD2	2:B:500:PLP:N1	2.52	0.43
1:D:212:PHE:CZ	1:D:271:LEU:HD22	2.54	0.42
1:B:251:LEU:CD1	1:B:294[B]:MSE:HE1	2.48	0.42
1:A:60:VAL:HG13	1:B:53:ASN:CB	2.49	0.42
1:A:241:VAL:HB	1:A:260:LEU:HB3	2.02	0.42
1:C:277:GLY:O	1:D:10:LEU:HD23	2.20	0.41
1:A:70:GLY:HA2	1:B:252:PRO:HG2	2.02	0.41
1:A:376:VAL:HB	1:A:380[A]:MSE:HE3	2.02	0.41
1:A:294[A]:MSE:CE	1:A:295:ILE:HD12	2.49	0.41
1:B:27:ARG:NH2	1:B:31:VAL:HG11	2.35	0.41
1:C:294[A]:MSE:SE	1:C:295:ILE:HD12	2.71	0.41
1:B:222:ILE:HD11	1:B:247:LYS:HB3	2.03	0.40
1:D:214:ILE:HD12	1:D:214:ILE:N	2.36	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	400/398 (100%)	387 (97%)	12 (3%)	1 (0%)	46	45
1	B	400/398 (100%)	385 (96%)	14 (4%)	1 (0%)	46	45
1	C	402/398 (101%)	386 (96%)	16 (4%)	0	100	100
1	D	401/398 (101%)	386 (96%)	14 (4%)	1 (0%)	52	53
All	All	1603/1592 (101%)	1544 (96%)	56 (4%)	3 (0%)	52	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	GLU
1	B	217	GLU
1	D	217	GLU

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	335/325 (103%)	330 (98%)	5 (2%)	72	78
1	B	334/325 (103%)	329 (98%)	5 (2%)	72	78
1	C	333/325 (102%)	330 (99%)	3 (1%)	84	89
1	D	329/325 (101%)	327 (99%)	2 (1%)	90	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1331/1300 (102%)	1316 (99%)	15 (1%)	80 85

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	PRO
1	A	295	ILE
1	A	333	PHE
1	A	362	ASP
1	A	366	CYS
1	B	183	PRO
1	B	205	LYS
1	B	333	PHE
1	B	336	PHE
1	B	344	SER
1	C	183	PRO
1	C	317	GLU
1	C	362	ASP
1	D	336	PHE
1	D	344	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	PLP	A	500	-	16,16,16	1.39	4 (25%)	21,23,23	1.43	4 (19%)
3	EDO	A	501	-	3,3,3	0.39	0	2,2,2	0.61	0
3	EDO	A	502	-	3,3,3	0.41	0	2,2,2	0.46	0
2	PLP	B	500	-	16,16,16	1.31	2 (12%)	21,23,23	1.43	3 (14%)
3	EDO	B	502	-	3,3,3	0.46	0	2,2,2	0.55	0
3	EDO	B	503	-	3,3,3	0.49	0	2,2,2	0.29	0
3	EDO	B	504	-	3,3,3	0.45	0	2,2,2	0.55	0
3	EDO	B	505	-	3,3,3	0.61	0	2,2,2	0.25	0
3	EDO	B	506	-	3,3,3	0.54	0	2,2,2	0.38	0
3	EDO	B	507	-	3,3,3	0.53	0	2,2,2	0.09	0
3	EDO	B	508	-	3,3,3	0.31	0	2,2,2	0.57	0
3	EDO	B	509	-	3,3,3	0.41	0	2,2,2	0.18	0
3	EDO	B	510	-	3,3,3	0.40	0	2,2,2	0.35	0
2	PLP	C	500	-	16,16,16	1.29	2 (12%)	21,23,23	1.21	3 (14%)
3	EDO	C	501	-	3,3,3	0.44	0	2,2,2	0.11	0
2	PLP	D	500	-	16,16,16	1.24	3 (18%)	21,23,23	1.26	3 (14%)

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	PLP	A	500	-	-	0/8/8/8	0/1/1/1
3	EDO	A	501	-	-	0/1/1/1	0/0/0/0
3	EDO	A	502	-	-	0/1/1/1	0/0/0/0
2	PLP	B	500	-	-	0/8/8/8	0/1/1/1
3	EDO	B	502	-	-	0/1/1/1	0/0/0/0
3	EDO	B	503	-	-	0/1/1/1	0/0/0/0
3	EDO	B	504	-	-	0/1/1/1	0/0/0/0
3	EDO	B	505	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	506	-	-	0/1/1/1	0/0/0/0
3	EDO	B	507	-	-	0/1/1/1	0/0/0/0
3	EDO	B	508	-	-	0/1/1/1	0/0/0/0
3	EDO	B	509	-	-	0/1/1/1	0/0/0/0
3	EDO	B	510	-	-	0/1/1/1	0/0/0/0
2	PLP	C	500	-	-	0/8/8/8	0/1/1/1
3	EDO	C	501	-	-	0/1/1/1	0/0/0/0
2	PLP	D	500	-	-	0/8/8/8	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	PLP	C6-C5	2.04	1.42	1.37
2	A	500	PLP	C6-N1	2.10	1.39	1.34
2	D	500	PLP	C6-N1	2.17	1.39	1.34
2	B	500	PLP	C4-C4A	2.24	1.51	1.46
2	C	500	PLP	C2-N1	2.40	1.39	1.34
2	A	500	PLP	C4-C4A	2.46	1.52	1.46
2	D	500	PLP	C4-C4A	2.46	1.52	1.46
2	D	500	PLP	C2-N1	2.76	1.39	1.34
2	C	500	PLP	C4-C4A	2.83	1.53	1.46
2	A	500	PLP	C2-N1	2.85	1.40	1.34
2	B	500	PLP	C2-N1	2.87	1.40	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	500	PLP	C5-C6-N1	-2.95	118.74	123.86
2	B	500	PLP	O4A-C4A-C4	-2.59	119.88	125.11
2	A	500	PLP	O4A-C4A-C4	-2.53	120.01	125.11
2	A	500	PLP	C3-C4-C4A	-2.51	116.05	119.84
2	A	500	PLP	C5-C6-N1	-2.44	119.62	123.86
2	C	500	PLP	C5-C6-N1	-2.38	119.72	123.86
2	D	500	PLP	O4A-C4A-C4	-2.29	120.48	125.11
2	D	500	PLP	C5-C6-N1	-2.09	120.23	123.86
2	C	500	PLP	C5A-C5-C6	-2.04	115.42	119.28
2	C	500	PLP	O4P-P-O1P	2.31	113.02	107.14
2	D	500	PLP	O4P-C5A-C5	2.48	113.09	108.99
2	A	500	PLP	O4P-C5A-C5	2.86	113.72	108.99
2	B	500	PLP	O4P-C5A-C5	3.72	115.14	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	PLP	1	0
2	B	500	PLP	2	0
2	D	500	PLP	1	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	390/398 (97%)	0.48	21 (5%)	29	38	29, 35, 45, 55	0
1	B	390/398 (97%)	0.55	22 (5%)	28	36	29, 35, 47, 63	0
1	C	389/398 (97%)	0.87	58 (14%)	3	5	28, 35, 46, 59	0
1	D	390/398 (97%)	0.87	46 (11%)	6	8	29, 35, 44, 59	0
All	All	1559/1592 (97%)	0.69	147 (9%)	11	14	28, 35, 45, 63	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	397	LYS	6.7
1	A	0	GLY	5.6
1	C	60	VAL	5.0
1	D	241	VAL	4.8
1	B	397	LYS	4.8
1	C	242	CYS	4.5
1	D	393	LYS	4.4
1	D	60	VAL	4.4
1	C	256	ILE	4.3
1	A	29	ALA	4.3
1	D	51	ILE	4.2
1	C	303	GLY	4.2
1	D	46	ILE	4.1
1	C	41	ILE	4.1
1	C	107	ALA	4.0
1	D	214	ILE	4.0
1	D	48	ALA	3.9
1	C	13	VAL	3.7
1	B	241	VAL	3.6
1	D	225	ASP	3.6
1	C	241	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	177	ILE	3.5
1	C	63	TYR	3.4
1	D	63	TYR	3.4
1	D	396	ASN	3.4
1	C	243	TYR	3.4
1	C	106	GLY	3.4
1	B	41	ILE	3.3
1	C	51	ILE	3.3
1	D	302	THR	3.3
1	C	111	LEU	3.3
1	D	53	ASN	3.3
1	C	215	ALA	3.3
1	C	21	PHE	3.2
1	B	19	GLU	3.2
1	D	215	ALA	3.2
1	C	12	SER	3.2
1	D	176	ILE	3.2
1	C	46	ILE	3.1
1	D	240	LEU	3.1
1	D	106	GLY	3.1
1	C	377	ASP	3.1
1	D	342	ASP	3.1
1	D	296	VAL	3.0
1	B	240	LEU	3.0
1	C	72	THR	3.0
1	C	214	ILE	3.0
1	B	16	ALA	3.0
1	A	256	ILE	2.9
1	C	257	GLY	2.9
1	C	18	ARG	2.8
1	A	26	LYS	2.8
1	D	177	ILE	2.8
1	B	215	ALA	2.8
1	C	258	TYR	2.8
1	D	109	ALA	2.8
1	C	59	LEU	2.8
1	C	53	ASN	2.8
1	A	242	CYS	2.8
1	B	214	ILE	2.8
1	A	60	VAL	2.8
1	A	215	ALA	2.8
1	D	242	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	321	ARG	2.8
1	D	213	ILE	2.8
1	D	395	TYR	2.7
1	C	259	VAL	2.7
1	B	110	SER	2.7
1	D	258	TYR	2.7
1	D	256	ILE	2.7
1	A	34	GLU	2.7
1	A	214	ILE	2.6
1	C	176	ILE	2.6
1	C	50	GLN	2.6
1	B	242	CYS	2.6
1	C	62	ASP	2.6
1	D	62	ASP	2.6
1	C	154	THR	2.6
1	A	241	VAL	2.6
1	D	13	VAL	2.6
1	C	87	PHE	2.6
1	C	314	LEU	2.5
1	C	16	ALA	2.5
1	D	259	VAL	2.5
1	A	240	LEU	2.5
1	B	377	ASP	2.5
1	C	108	ALA	2.5
1	C	66	VAL	2.5
1	C	295	ILE	2.5
1	D	223	VAL	2.5
1	C	97	ASN	2.4
1	A	63	TYR	2.4
1	A	41	ILE	2.4
1	A	155	GLU	2.4
1	C	218	PRO	2.3
1	D	301	ALA	2.3
1	D	201	GLU	2.3
1	C	95[A]	HIS	2.3
1	B	109	ALA	2.3
1	D	66	VAL	2.3
1	A	195	LYS	2.3
1	C	22	GLU	2.3
1	C	302	THR	2.3
1	A	66	VAL	2.3
1	C	110	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	52	VAL	2.3
1	C	43	ASN	2.3
1	C	301	ALA	2.3
1	A	257	GLY	2.2
1	A	243	TYR	2.2
1	C	155[A]	GLU	2.2
1	D	0	GLY	2.2
1	B	21	PHE	2.2
1	D	31	VAL	2.2
1	D	232	VAL	2.2
1	B	25	LYS	2.2
1	D	57	LYS	2.2
1	B	111	LEU	2.2
1	D	64	ASP	2.2
1	D	52	VAL	2.2
1	D	306	ASN	2.2
1	B	20	LEU	2.1
1	B	22	GLU	2.1
1	A	387	ALA	2.1
1	C	48	ALA	2.1
1	D	288	PRO	2.1
1	B	176	ILE	2.1
1	A	57	LYS	2.1
1	C	216	ASP	2.1
1	C	260	LEU	2.1
1	C	55	THR	2.1
1	D	303	GLY	2.1
1	A	337	VAL	2.1
1	C	228	LYS	2.1
1	D	304	ASP	2.1
1	D	260	LEU	2.1
1	C	396	ASN	2.1
1	B	213	ILE	2.0
1	C	85	ALA	2.0
1	C	58	GLU	2.0
1	C	397	LYS	2.0
1	B	15	SER	2.0
1	D	59	LEU	2.0
1	C	14	ARG	2.0
1	C	133	PHE	2.0
1	B	256	ILE	2.0
1	D	227	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (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
3	EDO	B	503	4/4	0.84	0.23	7.21	38,41,43,48	0
3	EDO	A	502	4/4	0.92	0.29	5.18	59,59,60,62	0
3	EDO	B	508	4/4	0.84	0.31	4.80	55,56,58,59	0
3	EDO	B	504	4/4	0.88	0.19	4.33	34,38,41,49	0
2	PLP	D	500	16/16	0.73	0.26	1.91	60,65,70,72	0
3	EDO	B	502	4/4	0.89	0.17	1.12	32,38,39,40	0
3	EDO	C	501	4/4	0.83	0.24	0.92	58,58,58,60	0
3	EDO	A	501	4/4	0.94	0.16	0.54	28,38,40,41	0
3	EDO	B	505	4/4	0.86	0.18	0.31	36,44,46,50	0
2	PLP	C	500	16/16	0.82	0.21	-0.10	50,54,60,60	0
2	PLP	A	500	16/16	0.90	0.17	-0.11	30,38,49,55	0
3	EDO	B	506	4/4	0.90	0.15	-0.33	34,38,38,39	0
2	PLP	B	500	16/16	0.95	0.13	-1.16	33,40,48,55	0
3	EDO	B	507	4/4	0.87	0.29	-	47,51,51,55	0
3	EDO	B	510	4/4	0.89	0.16	-	51,51,53,55	0
4	CL	B	501	1/1	0.99	0.05	-	22,22,22,22	0
4	CL	D	501	1/1	0.98	0.09	-	32,32,32,32	0
3	EDO	B	509	4/4	0.85	0.17	-	54,56,56,56	0

6.5 Other polymers (i)

There are no such residues in this entry.