wwPDB X-ray Structure Validation Summary Report (i)

May 23, 2020 – 04:24 pm BST

PDB ID	:	2XH0
Title	:	Engineering the enolase active site pocket: Crystal structure of the S39N Q167K D321R mutant of yeast enolase 1
Authors	:	Schreier, B.; Hocker, B.
Deposited on	:	2010-06-08
Resolution	:	1.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/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:

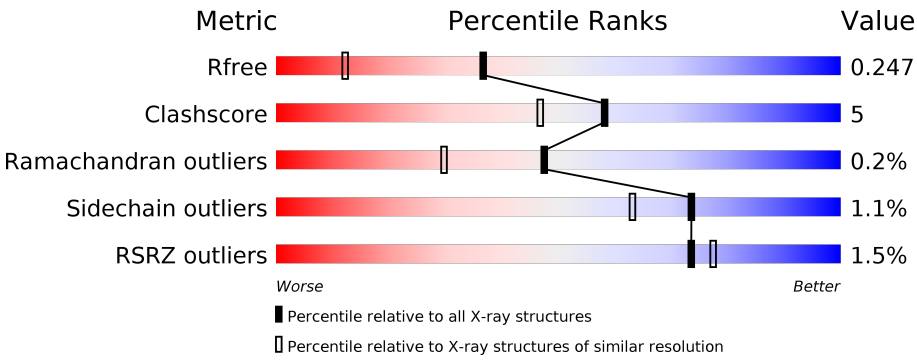
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 respectively. 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	443	87% 12% •
1	B	443	2% 87% 12% •
1	C	443	88% 10% •
1	D	443	2% 88% 10% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14787 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 ENOLASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	438	3310	2092	578	636	4	0	4	1
1	B	438	3272	2067	569	630	6	0	2	1
1	C	438	3305	2089	577	635	4	0	3	1
1	D	438	3287	2077	573	631	6	0	2	1

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	437	LEU	-	expression tag	UNP P00924
A	438	HIS	-	expression tag	UNP P00924
A	439	HIS	-	expression tag	UNP P00924
A	440	HIS	-	expression tag	UNP P00924
A	441	HIS	-	expression tag	UNP P00924
A	442	HIS	-	expression tag	UNP P00924
A	443	HIS	-	expression tag	UNP P00924
A	39	ASN	SER	engineered mutation	UNP P00924
A	167	LYS	GLN	engineered mutation	UNP P00924
A	241	ILE	VAL	conflict	UNP P00924
A	321	ARG	ASP	engineered mutation	UNP P00924
B	437	LEU	-	expression tag	UNP P00924
B	438	HIS	-	expression tag	UNP P00924
B	439	HIS	-	expression tag	UNP P00924
B	440	HIS	-	expression tag	UNP P00924
B	441	HIS	-	expression tag	UNP P00924
B	442	HIS	-	expression tag	UNP P00924
B	443	HIS	-	expression tag	UNP P00924
B	39	ASN	SER	engineered mutation	UNP P00924
B	167	LYS	GLN	engineered mutation	UNP P00924
B	241	ILE	VAL	conflict	UNP P00924

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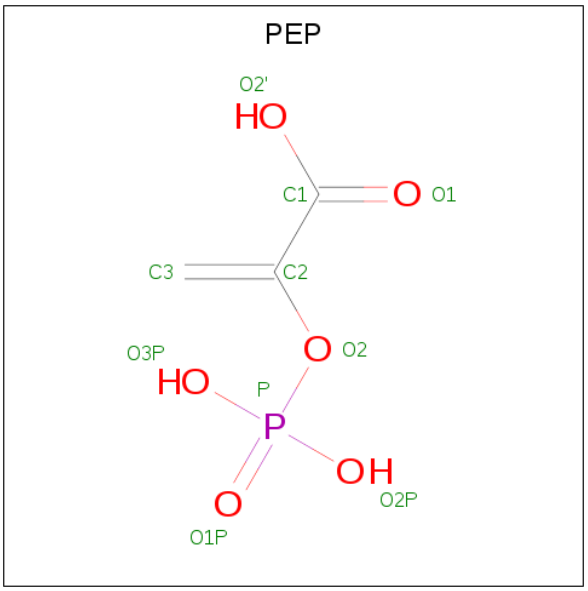
Chain	Residue	Modelled	Actual	Comment	Reference
B	321	ARG	ASP	engineered mutation	UNP P00924
C	437	LEU	-	expression tag	UNP P00924
C	438	HIS	-	expression tag	UNP P00924
C	439	HIS	-	expression tag	UNP P00924
C	440	HIS	-	expression tag	UNP P00924
C	441	HIS	-	expression tag	UNP P00924
C	442	HIS	-	expression tag	UNP P00924
C	443	HIS	-	expression tag	UNP P00924
C	39	ASN	SER	engineered mutation	UNP P00924
C	167	LYS	GLN	engineered mutation	UNP P00924
C	241	ILE	VAL	conflict	UNP P00924
C	321	ARG	ASP	engineered mutation	UNP P00924
D	437	LEU	-	expression tag	UNP P00924
D	438	HIS	-	expression tag	UNP P00924
D	439	HIS	-	expression tag	UNP P00924
D	440	HIS	-	expression tag	UNP P00924
D	441	HIS	-	expression tag	UNP P00924
D	442	HIS	-	expression tag	UNP P00924
D	443	HIS	-	expression tag	UNP P00924
D	39	ASN	SER	engineered mutation	UNP P00924
D	167	LYS	GLN	engineered mutation	UNP P00924
D	241	ILE	VAL	conflict	UNP P00924
D	321	ARG	ASP	engineered mutation	UNP P00924

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0

- Molecule 3 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula: $C_3H_5O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
3	A	1	10	3	6	1	0	0
			Total	C	O	P		
3	B	1	10	3	6	1	0	0
			Total	C	O	P		
3	C	1	10	3	6	1	0	0
			Total	C	O	P		
3	D	1	10	3	6	1	0	0

- Molecule 4 is water.

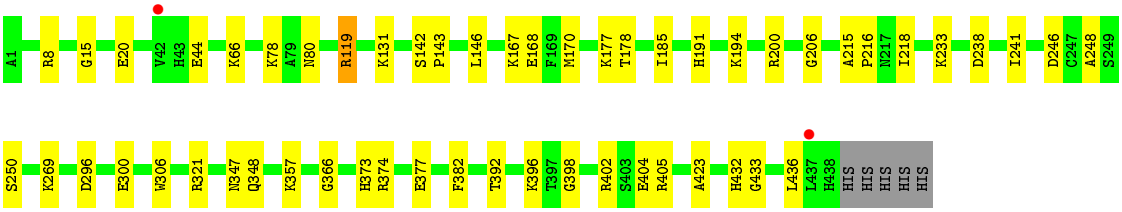
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	449	449	449	0	0
			Total	O		
4	B	411	411	411	0	0
			Total	O		
4	C	405	405	405	0	0
			Total	O		
4	D	304	304	304	0	0

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 the various outlier classes 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.

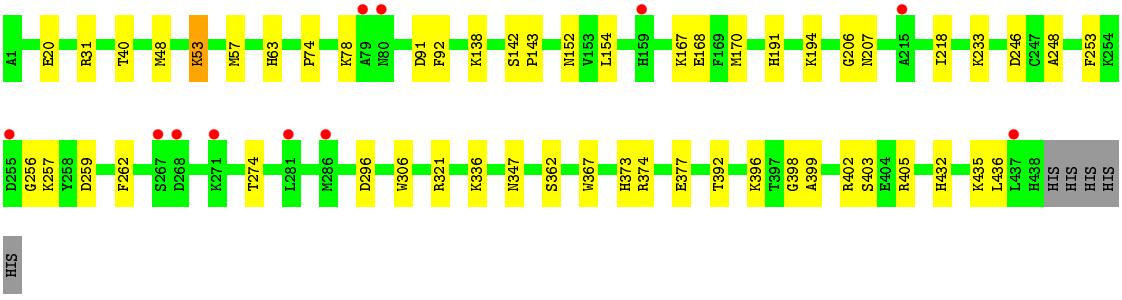
- Molecule 1: ENOLASE 1

Chain A:



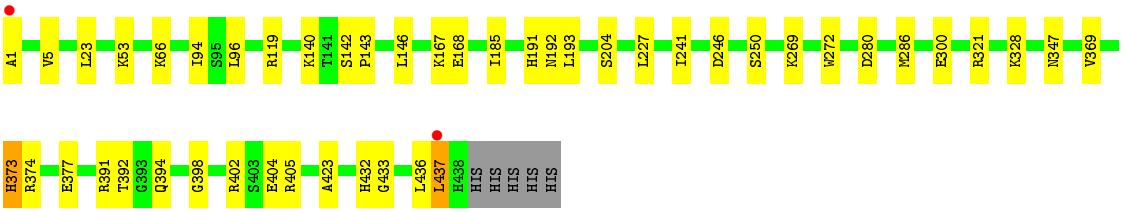
- Molecule 1: ENOLASE 1

Chain B:



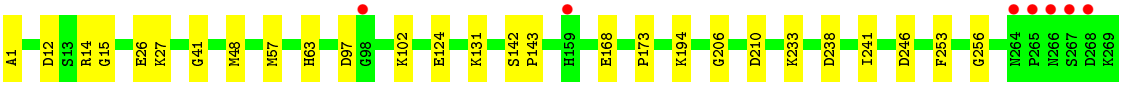
- Molecule 1: ENOLASE 1

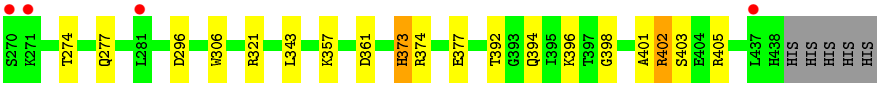
Chain C:



- Molecule 1: ENOLASE 1

Chain D:


A1
D12
S13
R14
G15
E26
K27
G41
M48
M57
H63
D97
G98
K102
E124
K131
S142
P143
H159
E168
P173
K194
G206
D210
K233
D238
I241
D246
F253
G256
N264
P265
N266
S267
D268
K269


S270
K271
T274
Q277
L281
D296
W306
R321
L343
K357
D361
H373
R374
E377
T392
G393
Q394
I395
K396
T397
G398
A401
R402
S403
E404
R405
L437
H438
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	55.33Å 60.80Å 120.67Å 89.89° 89.90° 65.84°	Depositor
Resolution (Å)	37.85 – 1.70 37.84 – 1.70	Depositor EDS
% Data completeness (in resolution range)	93.2 (37.85-1.70) 76.1 (37.84-1.70)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.197 , 0.246 0.198 , 0.247	Depositor DCC
R_{free} test set	6059 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	12.6	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 42.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.147 for h,h-k,-l 0.459 for -h,-k,l 0.147 for -h,-h+k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14787	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.82% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.53	0/3382	0.66	2/4579 (0.0%)
1	B	0.52	0/3338	0.65	0/4528
1	C	0.53	0/3374	0.65	1/4568 (0.0%)
1	D	0.52	0/3353	0.65	1/4544 (0.0%)
All	All	0.52	0/13447	0.66	4/18219 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	119	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	D	12	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	119	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	C	119	ARG	NE-CZ-NH2	-5.03	117.78	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	3310	0	3323	34	0
1	B	3272	0	3238	37	0
1	C	3305	0	3317	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3287	0	3275	27	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	10	0	2	0	0
3	B	10	0	2	0	0
3	C	10	0	2	0	0
3	D	10	0	2	0	0
4	A	449	0	0	5	0
4	B	411	0	0	10	1
4	C	405	0	0	10	0
4	D	304	0	0	3	0
All	All	14787	0	13161	126	1

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 5.

The worst 5 of 126 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:369:VAL:O	1:C:392:THR:CG2	2.10	0.98
1:C:369:VAL:O	1:C:392:THR:HG23	1.69	0.90
1:C:300:GLU:HG2	1:C:321:ARG:HB3	1.57	0.86
1:B:194:LYS:HE3	4:B:2239:HOH:O	1.78	0.81
1:A:131:LYS:HE2	4:A:2227:HOH:O	1.86	0.74

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2124:HOH:O	4:B:2263:HOH:O[1_565]	1.93	0.27

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	440/443 (99%)	432 (98%)	7 (2%)	1 (0%)	47	30
1	B	438/443 (99%)	429 (98%)	8 (2%)	1 (0%)	47	30
1	C	439/443 (99%)	431 (98%)	7 (2%)	1 (0%)	47	30
1	D	438/443 (99%)	427 (98%)	10 (2%)	1 (0%)	47	30
All	All	1755/1772 (99%)	1719 (98%)	32 (2%)	4 (0%)	47	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	402	ARG
1	B	402	ARG
1	C	402	ARG
1	D	402	ARG

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	345/351 (98%)	341 (99%)	4 (1%)	71	59
1	B	335/351 (95%)	331 (99%)	4 (1%)	71	59
1	C	344/351 (98%)	340 (99%)	4 (1%)	71	59
1	D	339/351 (97%)	336 (99%)	3 (1%)	78	70
All	All	1363/1404 (97%)	1348 (99%)	15 (1%)	73	63

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	373	HIS
1	B	392	THR
1	D	373	HIS

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Mol	Chain	Res	Type
1	B	347	ASN
1	C	437	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	155	ASN
1	C	192	ASN
1	D	316	GLN
1	C	152	ASN
1	D	277	GLN

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
3	PEP	C	1440	2	6,9,9	1.53	1 (16%)	8,13,13	1.75	3 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PEP	B	1440	2	6,9,9	1.47	1 (16%)	8,13,13	1.17	1 (12%)
3	PEP	D	1440	2	6,9,9	1.33	1 (16%)	8,13,13	1.21	1 (12%)
3	PEP	A	1440	2	6,9,9	1.35	1 (16%)	8,13,13	1.81	2 (25%)

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	PEP	C	1440	2	-	0/5/9/9	-
3	PEP	B	1440	2	-	1/5/9/9	-
3	PEP	D	1440	2	-	0/5/9/9	-
3	PEP	A	1440	2	-	0/5/9/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1440	PEP	C3-C2	2.78	1.38	1.33
3	D	1440	PEP	C3-C2	2.58	1.38	1.33
3	C	1440	PEP	C3-C2	2.52	1.37	1.33
3	A	1440	PEP	C3-C2	2.40	1.37	1.33

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1440	PEP	O2-C2-C3	-3.37	118.30	124.79
3	C	1440	PEP	O2-C2-C3	-3.15	118.73	124.79
3	A	1440	PEP	O2-P-O1P	-2.95	98.84	109.32
3	B	1440	PEP	O2-C2-C3	-2.54	119.89	124.79
3	D	1440	PEP	O2-C2-C3	-2.37	120.23	124.79

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1440	PEP	C3-C2-O2-P

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	438/443 (98%)	0.05	2 (0%)	91	92	6, 13, 21, 32	0
1	B	438/443 (98%)	0.20	11 (2%)	57	61	6, 14, 26, 44	0
1	C	438/443 (98%)	0.01	2 (0%)	91	92	6, 13, 21, 31	0
1	D	438/443 (98%)	0.15	11 (2%)	57	61	6, 13, 24, 45	0
All	All	1752/1772 (98%)	0.10	26 (1%)	73	77	6, 13, 23, 45	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	437	LEU	4.3
1	D	266	ASN	3.7
1	D	265	PRO	3.7
1	B	159	HIS	3.6
1	C	1	ALA	3.3

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. 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	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PEP	B	1440	10/10	0.97	0.10	10,14,17,17	0
3	PEP	D	1440	10/10	0.97	0.10	12,18,22,23	0
3	PEP	A	1440	10/10	0.97	0.06	10,13,15,16	0
3	PEP	C	1440	10/10	0.98	0.08	8,12,15,17	0
2	MG	D	1439	1/1	0.98	0.14	2,2,2,2	0
2	MG	B	1439	1/1	0.99	0.14	2,2,2,2	0
2	MG	A	1439	1/1	0.99	0.14	2,2,2,2	0
2	MG	C	1439	1/1	1.00	0.16	2,2,2,2	0

6.5 Other polymers (i)

There are no such residues in this entry.