Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:17 PM GMT

PDB ID	:	1EUD
Title	:	CRYSTAL STRUCTURE OF PHOSPHORYLATED PIG HEART, GTP-SPECIFIC SUCCINYL-COA SYNTHETASE
Authors	:	Fraser, M.E.; James, M.N.G.; Bridger, W.A.; Wolodko, W.T.
Deposited on	:	2000-04-14
Resolution	:	2.10 Å(reported)

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.
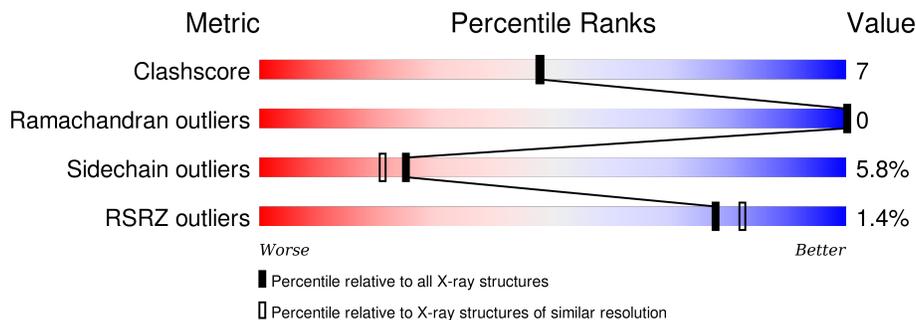
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	311	88% · · 9%
2	B	396	2% 80% 18% ·

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	SO4	B	396	-	-	-	X
3	SO4	B	397	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5451 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 SUCCINYL-COA SYNTHETASE, ALPHA CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	306	Total 2262	C 1421	N 401	O 426	P 1	S 13	0	1	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	CLONING ARTIFACT	GB 2258465
A	-3	ALA	-	CLONING ARTIFACT	GB 2258465
A	259	NEP	HIS	MODIFIED RESIDUE	GB 2258465

- Molecule 2 is a protein called SUCCINYL-COA SYNTHETASE, BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	395	Total 2991	C 1889	N 505	O 581	S 16	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	CLONING ARTIFACT	UNP P53590
B	1	VAL	LEU	ENGINEERED	UNP P53590
B	332	CME	CYS	MODIFIED RESIDUE	UNP P53590
B	343	CSS	CYS	MODIFIED RESIDUE	UNP P53590

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
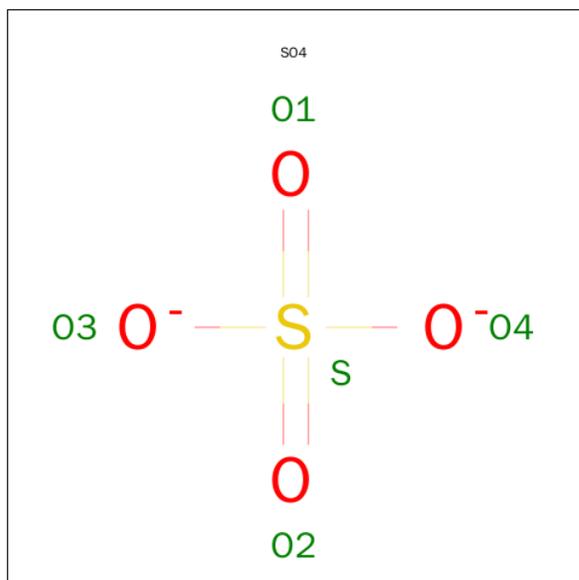
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	115	Total 115	O 115	0	0
4	B	73	Total 73	O 73	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: SUCCINYL-COA SYNTHETASE, ALPHA CHAIN

Chain A:
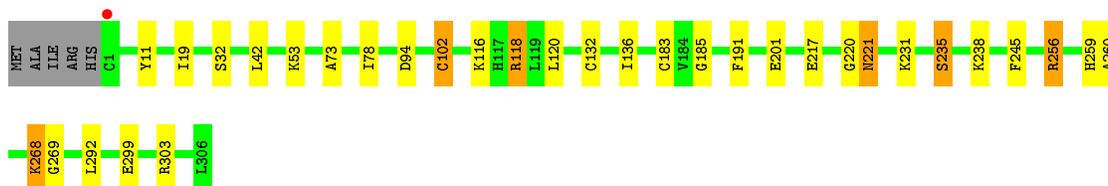
• Molecule 2: SUCCINYL-COA SYNTHETASE, BETA CHAIN

Chain B:
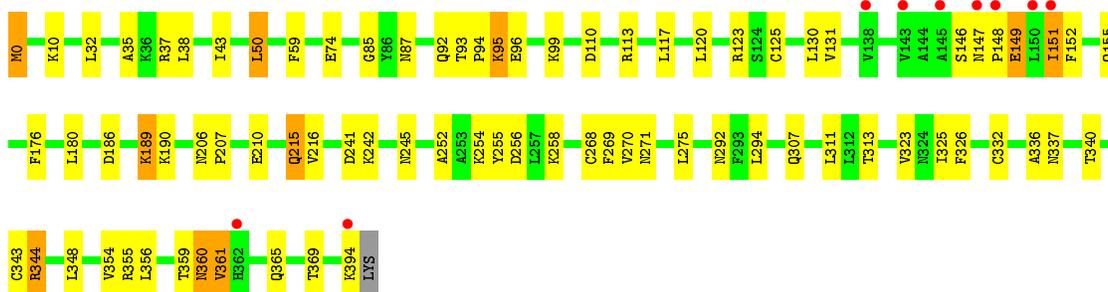
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.91Å 82.28Å 50.02Å 90.00° 104.37° 90.00°	Depositor
Resolution (Å)	41.00 – 2.10 41.14 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.9 (41.00-2.10) 97.9 (41.14-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 2.10Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.156 , 0.215 0.172 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	21.1	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 56.9	EDS
Estimated twinning fraction	0.028 for -h-l,-k,l	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 39063 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5451	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: CSS, CME, SO4, NEP

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	0.90	2/2293 (0.1%)	0.90	0/3097
2	B	0.80	1/3009 (0.0%)	0.90	0/4058
All	All	0.84	3/5302 (0.1%)	0.90	0/7155

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	268	CYS	CB-SG	-6.19	1.71	1.82
1	A	102	CYS	CB-SG	-5.39	1.73	1.81
1	A	201	GLU	CG-CD	-5.14	1.44	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2262	0	2304	28	0
2	B	2991	0	3049	51	0
3	B	10	0	0	0	0
4	A	115	0	0	0	0
4	B	73	0	0	3	0
All	All	5451	0	5353	78	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 7.

All (78) 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:A:118:ARG:HH11	1:A:118:ARG:HB3	1.22	1.00
1:A:118:ARG:HH11	1:A:118:ARG:CB	1.83	0.91
2:B:95:LYS:HE2	2:B:95:LYS:H	1.42	0.84
1:A:118:ARG:HH11	1:A:118:ARG:CG	1.97	0.77
1:A:118:ARG:HB3	1:A:118:ARG:NH1	2.00	0.76
2:B:147:ASN:HA	2:B:149:GLU:OE2	1.88	0.74
2:B:361:VAL:O	2:B:365:GLN:HG2	1.92	0.70
2:B:344:ARG:HH11	2:B:344:ARG:CB	2.06	0.69
2:B:210:GLU:HA	2:B:215:GLN:O	2.00	0.60
2:B:343:CSS:SD	2:B:348:LEU:HB2	2.43	0.58
2:B:340:THR:O	2:B:344:ARG:HD3	2.04	0.58
2:B:148:PRO:O	2:B:151:ILE:HG23	2.03	0.58
1:A:245:PHE:HB2	1:A:292:LEU:HD21	1.86	0.57
1:A:299:GLU:O	1:A:303:ARG:HG2	2.05	0.56
2:B:252:ALA:HB2	2:B:311:LEU:HD21	1.88	0.56
2:B:35:ALA:HB1	2:B:43:ILE:HD13	1.86	0.55
1:A:268:LYS:HE3	1:A:269:GLY:N	2.22	0.55
2:B:215:GLN:HE21	2:B:215:GLN:HA	1.72	0.55
2:B:215:GLN:HE21	2:B:215:GLN:CA	2.19	0.54
2:B:255:TYR:O	2:B:256:ASP:HB2	2.08	0.53
2:B:147:ASN:CA	2:B:149:GLU:OE2	2.56	0.52
1:A:94:ASP:OD1	1:A:118:ARG:NH2	2.43	0.52
1:A:116:LYS:O	1:A:120:LEU:HG	2.09	0.52
2:B:215:GLN:NE2	2:B:215:GLN:HA	2.25	0.51
1:A:32:SER:HB3	1:A:42:LEU:HD21	1.92	0.51
2:B:270:VAL:HG11	2:B:275:LEU:HG	1.93	0.51
1:A:118:ARG:CG	1:A:118:ARG:NH1	2.64	0.51
2:B:344:ARG:HH11	2:B:344:ARG:HB2	1.75	0.50
2:B:186:ASP:HA	2:B:189:LYS:HD3	1.94	0.50
2:B:151:ILE:HD12	2:B:152:PHE:N	2.27	0.50
2:B:131:VAL:HG13	2:B:151:ILE:CD1	2.41	0.49
2:B:113:ARG:HG3	4:B:451:HOH:O	2.13	0.49
2:B:96:GLU:H	2:B:96:GLU:CD	2.16	0.49
1:A:19:ILE:HG23	1:A:73:ALA:HB2	1.94	0.48
2:B:359:THR:HG22	2:B:360:ASN:HB2	1.94	0.48
1:A:221:ASN:C	1:A:221:ASN:HD22	2.16	0.48
1:A:191:PHE:CE1	2:B:123:ARG:HA	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:LYS:HA	2:B:245:ASN:ND2	2.29	0.47
2:B:258:LYS:O	2:B:294:LEU:HD12	2.13	0.47
1:A:221:ASN:ND2	1:A:221:ASN:C	2.68	0.47
2:B:252:ALA:CB	2:B:311:LEU:HD21	2.44	0.47
2:B:180:LEU:HD23	2:B:180:LEU:N	2.30	0.47
2:B:32:LEU:HD13	2:B:74:GLU:HA	1.97	0.46
1:A:118:ARG:HG2	1:A:118:ARG:HH11	1.78	0.46
1:A:32:SER:HB3	1:A:42:LEU:CD2	2.46	0.46
1:A:231:LYS:O	1:A:235:SER:HB2	2.17	0.45
1:A:118:ARG:HG2	1:A:118:ARG:NH1	2.32	0.45
1:A:220:GLY:O	1:A:268:LYS:HE2	2.16	0.45
2:B:270:VAL:CG1	2:B:275:LEU:HG	2.47	0.45
2:B:125:CYS:HB3	2:B:155:GLN:HE21	1.82	0.44
2:B:85:GLY:O	2:B:99:LYS:HE2	2.17	0.44
2:B:206:ASN:HA	2:B:207:PRO:HA	1.80	0.44
2:B:37:ARG:O	2:B:38:LEU:C	2.55	0.43
2:B:113:ARG:CG	4:B:451:HOH:O	2.66	0.43
2:B:254:LYS:HB3	2:B:254:LYS:HE3	1.78	0.43
2:B:255:TYR:CE2	2:B:307:GLN:NE2	2.87	0.43
2:B:35:ALA:HB1	2:B:43:ILE:CD1	2.49	0.43
2:B:325:ILE:HG22	2:B:332:CME:HZ3	2.00	0.43
2:B:93:THR:C	2:B:94:PRO:O	2.56	0.43
2:B:50:LEU:HD21	2:B:241:ASP:HB3	2.01	0.42
2:B:292:ASN:ND2	2:B:294:LEU:HB2	2.34	0.42
1:A:78:ILE:HB	1:A:102:CYS:HA	2.00	0.42
1:A:136:ILE:HG22	1:A:183[B]:CYS:HB3	2.02	0.42
2:B:151:ILE:C	2:B:151:ILE:HD12	2.40	0.42
2:B:271:ASN:OD1	2:B:325:ILE:HA	2.18	0.42
1:A:256:ARG:CZ	1:A:256:ARG:HB3	2.49	0.42
2:B:59:PHE:HA	2:B:87:ASN:O	2.20	0.41
2:B:215:GLN:NE2	2:B:215:GLN:CA	2.83	0.41
2:B:354:VAL:HG12	2:B:356:LEU:HG	2.01	0.41
1:A:221:ASN:HD22	1:A:221:ASN:H	1.67	0.41
2:B:269:PHE:CZ	2:B:323:VAL:HG22	2.55	0.41
2:B:0:MET:HA	4:B:438:HOH:O	2.21	0.41
2:B:176:PHE:CE2	2:B:216:VAL:HG22	2.56	0.41
1:A:217:GLU:OE2	1:A:259:NEP:ND1	2.54	0.41
1:A:268:LYS:HE3	1:A:269:GLY:CA	2.51	0.41
1:A:132:CYS:HB2	1:A:185:GLY:O	2.21	0.40
2:B:336:ALA:O	2:B:340:THR:HG23	2.22	0.40
1:A:256:ARG:HD2	1:A:260:ALA:HA	2.03	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	304/311 (98%)	297 (98%)	7 (2%)	0	100	100
2	B	391/396 (99%)	385 (98%)	6 (2%)	0	100	100
All	All	695/707 (98%)	682 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	239/242 (99%)	231 (97%)	8 (3%)	45	47
2	B	317/318 (100%)	293 (92%)	24 (8%)	16	12
All	All	556/560 (99%)	524 (94%)	32 (6%)	25	21

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	TYR
1	A	53	LYS
1	A	118	ARG
1	A	221	ASN
1	A	235	SER

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Mol	Chain	Res	Type
1	A	238	LYS
1	A	256	ARG
1	A	268	LYS
2	B	0	MET
2	B	10	LYS
2	B	50	LEU
2	B	92	GLN
2	B	95	LYS
2	B	110	ASP
2	B	117	LEU
2	B	120	LEU
2	B	130	LEU
2	B	146	SER
2	B	149	GLU
2	B	151	ILE
2	B	189	LYS
2	B	190	LYS
2	B	215	GLN
2	B	313	THR
2	B	326	PHE
2	B	337	ASN
2	B	344	ARG
2	B	355	ARG
2	B	360	ASN
2	B	361	VAL
2	B	369	THR
2	B	394	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	ASN
1	A	225	ASN
1	A	232	GLN
1	A	233	HIS
1	A	279	GLN
2	B	135	GLN
2	B	147	ASN
2	B	155	GLN
2	B	168	GLN
2	B	182	ASN
2	B	215	GLN

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Mol	Chain	Res	Type
2	B	224	ASN
2	B	245	ASN
2	B	307	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)

3 non-standard protein/DNA/RNA residues 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	$\#|Z| > 2$
1	NEP	A	259	1	10,14,15	1.19	1 (10%)	4,20,22	1.75	1 (25%)
2	CME	B	332	2	8,9,10	0.59	0	6,9,11	1.08	1 (16%)
2	CSS	B	343	2	4,6,7	0.63	0	3,6,8	1.19	0

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
1	NEP	A	259	1	-	0/4/12/14	0/1/1/1
2	CME	B	332	2	-	0/5/8/10	0/0/0/0
2	CSS	B	343	2	-	0/1/5/7	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	259	NEP	P-O2P	-2.69	1.48	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	332	CME	O-C-CA	-2.20	119.77	125.49
1	A	259	NEP	O2P-P-O3P	2.68	120.58	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	259	NEP	1	0
2	B	332	CME	1	0
2	B	343	CSS	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	SO4	B	396	-	4,4,4	0.14	0	6,6,6	0.42	0
3	SO4	B	397	-	4,4,4	0.18	0	6,6,6	0.31	0

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	SO4	B	396	-	-	0/0/0/0	0/0/0/0
3	SO4	B	397	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (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(Å²)	Q<0.9
1	A	305/311 (98%)	-0.46	1 (0%)	94	95	10, 18, 39, 66	1 (0%)
2	B	393/396 (99%)	-0.32	9 (2%)	64	70	11, 28, 55, 71	0
All	All	698/707 (98%)	-0.38	10 (1%)	78	82	10, 23, 51, 71	1 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	394	LYS	4.3
1	A	1	CYS	4.0
2	B	362	HIS	3.0
2	B	145	ALA	2.6
2	B	150	LEU	2.6
2	B	148	PRO	2.4
2	B	151	ILE	2.4
2	B	147	ASN	2.3
2	B	138	VAL	2.1
2	B	143	VAL	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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, 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	LLDF	B-factors(Å²)	Q<0.9
1	NEP	A	259	14/15	0.99	0.12	-	14,18,24,24	0
2	CSS	B	343	7/8	0.97	0.06	-	29,33,34,48	0
2	CME	B	332	10/11	0.98	0.07	-	25,29,30,37	0

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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	B	396	5/5	0.95	0.24	10.32	25,26,27,28	5
3	SO4	B	397	5/5	0.96	0.32	6.33	27,31,33,33	5

6.5 Other polymers (i)

There are no such residues in this entry.